Plenary Lecture : **PLEN-1**
Plenary Lecture
Room 205 THU 13:30
Chair: Dongwhan Lee (Seoul National University)

A Journey to Molecular Excitonic World

Dongho Kim

Department of Chemistry, Yonsei University, Korea

Various synthetic strategies have been developed to devise a variety of artificial molecular arrays in molecular photonics because of their similarities in architecture and subunit structures to the natural photosynthetic light-harvesting complexes. For the molecular arrays to be efficient devices, they should have very regular pigment arrangements which allow a facile light energy or charge flow along the array but do not result in the alteration of individual properties of the constituent pigments leading to the formation of energy or charge sink. In these respects, understanding of photophysical properties of these macromolecular architectures is essential for the rational design of molecular devices for photovoltaic, or optoelectronic applications.Here, we have revealed that the ultrafast excitation energy migration processes in molecular arrays are strongly influenced by the electronic couplings among the constituent molecules as well as the structural rigidity of overall architectures. Our investigations have been extended to H-type aggregated perylenebisimide (PBI) and polythiophene oligomers (linear vs. cyclic). Not only intermolecular exciton couplings but intramolecular electronic structures have been investigated in a series of expanded porphyrins in conjunction with their molecular structures, the number of π-electrons (Hückel's [4n+2] rule) as well as their conjugation pathways. Our study demonstrates a relationship between the photophysical properties such as absorption/emission properties, excited state dynamics and the aromaticity of expanded porphyrin systems. Based on these spectroscopic observations, we have found the reversal of aromaticity in the excited states of aromatic/antiaromatic expanded porphyrin congeners.[4] Detailed studies of the modulation events are expected to provide additional fruitful insight into the relationship between (anti)aromaticity and electronic structures. To the extent this proves true, it could have far-reaching practical applications that complement the advances in theoretical understanding that our studies are likely to provide.

Award Lecture : **AWARD-1**
Award Lecture
Room 205 FRI 13:30
Chair: Eunsung Lee (POSTECH)

Postsynthetic modifications of metal–organic frameworks and their applications

Myoung Soo Lah

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

Stepwise approaches can be used to obtain a variety of metal–organic frameworks (MOFs) that are not attainable by one-pot solvothermal reaction. MOF-74 is one of the most explored MOFs, but its functionalization is limited to the dative post-synthetic modification (PSM) of the monodentate solvent site. Owing to the nature of the organic ligand and framework structure of MOF-74, the covalent PSM of MOF-74 is very demanding. The covalent PSM of the amino group of amino-tagged defective Ni-MOF-74, which is prepared by de novo solvothermal synthesis using aminosalicylic acid as a functionalized fragmented organic ligand, generates metal-binding sites, and subsequent post-synthetic metalation with Pd(II) ions affords Pd(II)-incorporated Ni-MOF-74 catalyst. This catalyst exhibits highly efficient, size-selective, and recyclable catalytic activity for the Suzuki–Miyaura cross-coupling reaction. Meanwhile, a MOF having superprotonic conductivity is prepared by dative PSM of MOF-808. The activation of the sulfamate (SA)-grafted MOF-808 changes the binding mode of the grafted SA from monodentate to bridging bidentate, thus converting the neutral amido (–S–NH2) moiety of the grafted SA to the more acidic cationic sulfiliminium (–S=NH2+) moiety. The MOF with sulfiliminium moiety is found to have a proton conductivity of 7.89 × 10-2 S/cm. Moreover, this superprotonic conductivity is well maintained over 1000 cycles of conductivity measurements and for similar cyclic measurements each day for seven days.

Symposium : **KCS1-1**
[KAIST-SRC Symposium] Frontiers in Multiscale Chirality
Room 101 WED 13:30
Chair: Myungeun Seo (KAIST)

Foldamer-Based Chiral Molecular Architectures

Hee-Seung Lee

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

Biomacromolecules are programmed to assemble hierarchical structures in a wide range of scales for primary biological functions. In addition, protein subunits are utilized in nature to construct more complex nano- to microstructures required for spatiotemporal operations. The morphologies and functional anisotropies of assemblies are essential factors to ensure higher-order, functional molecular systems. However, the design of 3D assemblies from peptidic scaffolds is a nontrivial subject in synthetic and material sciences because of the difficulties in morphology control of peptide assemblies. To our best knowledge, the noncovalent synthesis of hierarchical assemblies and the molecular design strategy for nondestructive morphology transformation from a given shape to other well-defined forms are unknown. Peptide foldamers are attractive molecular scaffolds that mimic protein-like assemblies by noncovalent synthesis because they can adopt well-defined secondary structures and be designed modularly to emulate the self-organizing behavior of biomacromolecules. This seminar will discuss molecular design strategies to construct chiral, complex, high-order molecular architectures from helical foldamers.

Symposium : **KCS1-2**
[KAIST-SRC Symposium] Frontiers in Multiscale Chirality
Room 101 WED 14:00
Chair: Myungeun Seo (KAIST)

Surface Coatings by Polyphenols and Phenolamines

Haeshin Lee

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

Catecholamines are found ubiquitously in nature. Wetting-resistant, adhesive foot-pads in mussels, neurotransmitters in the brain, melanin biopigments in the skin and eyes, squid beaks, and insect cuticles are the examples. In materials science, catecholamines have recently attracted significant attentions due to the unparalleled material-independent surface functionalization properties. The most well-known material is poly(dopamine) and other derivatives such as poly(norepinephrine), chitosan-catechol and others will be introduced. First, I would like to present that the assembly of catecholamine and polydopamine is based on a new inter-molecular interaction known as cation-pi. Subsequently, my talk will introduce a new concept of self-sealing which is similar yet different with conventional self-healing materials. The first example is vascular self-sealing with rapid binding of intrinsic blood serum proteins to adhesive chitosan-catechol conjugate. The second example is plant-inspired nanoparticle formulation called TANNylation. In this study, we show that the modification of protein and peptide therapeutics with tannic acid—a flavonoid found in plants that adheres to extracellular matrices, elastins and collagens—improves their ability to specifically target heart tissue. Via a simple intravenous injection route, now one can easily delivery protein/peptide therapeutics directly to heart tissues. Finally, biomedical applications using polydopamine surface chemistry focusing on mammalian/stem cell culture and theranostic applications will be briefly explained in this talk.

Symposium : **KCS1-3**
[KAIST-SRC Symposium] Frontiers in Multiscale Chirality
Room 101 WED 14:20
Chair: Myungeun Seo (KAIST)

Creating Highly Crystalline Nanoplate Foldecture from Short α-Amino Acid Peptides and Its Molecular-level Structural Analysis

Jintaek Gong

Center for Multiscale Chiral Architectures, Korea Advanced Institute of Science and Technology, Korea

Rigid β-peptide foldamers rapidly self-assemble into various topologically complex three-dimensional structures, and these can be applied as anisotropic core materials and biocompatible delivery vehicles. However, the creation of well-defined and useful foldamer architectures (foldectures) from short and flexible α-amino acid peptides remains a significant challenge. This presentation details a systematic investigation of the self-assembly properties of α-peptide heptamers designed to populate helical secondary structures and form hydrophobic interactions, which are known to trigger self-association pathways in natural systems by strategically incorporating 2-aminoisobutyric acid residues into a leucine-rich primary sequence. The reproducible formation of homogenous two-dimensional nanoscale plates from the designed peptides is observed. Nuclear magnetic resonance spectroscopy is employed to develop high-resolution solution-state structural model. X-ray and microcrystal electron diffractions are used to evaluate solid-state models, which exhibit high crystallinities of the nanoplate, thus confirming the self-assembly results. In this study, a molecular-level design is used to demonstrate that new and potentially useful self-assembling materials can be obtained from inexpensive and commercially available α-amino acid peptides, a previously recalcitrant substrate class.

Symposium : **KCS1-4**
[KAIST-SRC Symposium] Frontiers in Multiscale Chirality
Room 101 WED 14:50
Chair: Myungeun Seo (KAIST)

Plasmonic Hybrid Nanoarchitectures for Boosting Light-to-Chemical Energy Conversion

Sang Woo Han

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

Light-to-chemical energy conversion based on plasmonic hybrid nanoarchitectures is a highly evolved scientific and industrial enterprise. For instance, it has recently been suggested that charge carriers either transferred directly from a photo-excited plasmonic metal nanostructure to an adjacent semiconductor, or induced by the plasmon energy transfer from a plasmonic nanostructure, could boost the efficiency of solar energy conversion processes, leading to a totally new paradigm in harvesting solar energy for practical use. To fully exploit the plasmonic function of heteronanostructures and thus to devise innovative solar energy conversion platforms, both the development of a rational strategy that can enable precise control over the topology of heteronanostructures and the elucidation of the underpinning mechanism of solar energy conversion processes are highly demanding. Here recently developed novel synthetic strategies to the realization of plasmonic hybrid nanoarchitectures with desired configurations and their use in plasmon-enhanced catalysis are reported. The prepared hybrid nanoarchitectures could enable the drastic elevation of solar energy conversion efficiency as well as the elucidation of the underlying mechanism of the plasmon-enhanced catalysis.

Symposium : **KCS1-5**
[KAIST-SRC Symposium] Frontiers in Multiscale Chirality
Room 101 WED 15:10
Chair: Myungeun Seo (KAIST)

Light-driven fabrication of helical nanostructures for optical applications

Dong Ki Yoon

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

Chiral liquid crystal phases show fascinating structural and optical properties due to the inherent helical characteristics. Among various kinds of chiral LC phases, the helical nanofilament phase made of achiral bent-shaped molecules has been in keen interest due to its unusual polar and chiral properties. This talk is intended to introduce the recent progress in the orientation control and its application of the HNF phase, which includes the photoalignment of the HNF phase, and chiroptical applications such as photonic crystal, chirality sensor, and security use. In detail, irradiating a film comprising azobenzene derivatives with UV light produces oriented arrays of HNFs via the photoisomerization-induced Weigert effect. As a result, structural colors are observed due to the extrinsic chiral reflection in the visible wavelength range, and the reflected color can be tuned by adjusting the molecular length of the azobenzene derivative. We also have directly visualized the optical activity of chiral samples using orientation-controlled HNFs. Right- or left-handed domains of the HNFs are large enough to be seen with the naked eye, up to ~several mm2. The periodic arrays of aligned HNFs reflect a specific color, here green, due to the Bragg reflection. Such a reflector enables easy detection of the optical activity of a sample placed on it. The device was tested with naturally chiral substances, like fructose and glucose, which exhibit an opposite sense of optical activity, as well as with structurally chiral nematic LC phase and revealed high sensitivity of detection. Indeed, we demonstrated security codes based on chiral photonic crystals made of HNFs that are not easy to be mimicked, which is quite different from the conventional technology used currently.

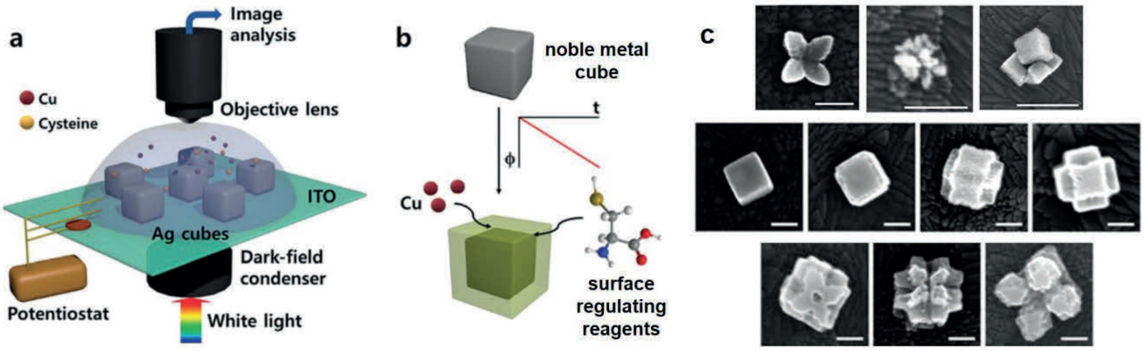
Symposium : **KCS1-6**
[KAIST-SRC Symposium] Frontiers in Multiscale Chirality
Room 101 WED 15:30
Chair: Myungeun Seo (KAIST)

Structural Complexity Manifested during Electrodeposition of Heterometals

Hyunjoon Song

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

Morphology evolution into intricate structures at the nanoscale is hard to understand, but we can get critical information from the combination of ex-situ and in-situ spectroelectrochemical techniques. We expect that electrodeposition can induce structural complexity by potential gradients formed through electrolytes. In contrast, wet chemical synthesis generates symmetrical structures by stirring the reaction mixture to adjust constant reagent concentrations. In this presentation, we will show the structural complexity generated during electrochemical Copper deposition on individual noble metal nanocrystals. Interestingly, complex and diverse morphologies have been manifested from simple cubic to clover- and octapod-like and branched. These structures are highly sensitive to the deposition conditions; precursor concentration, original surface morphology, seed density, potential sweep rate, and surface regulating reagent concentration. We try to understand the deposition mechanism using in-situ plasmon scattering with dark-field spectroscopy and explore the underpotential deposition inducing selective nucleation on the heterometal surfaces. Despite being diverse and sophisticated, all morphologies maintain their highly symmetric nature originating from pristine seed structures. These findings would be essential to design complex morphologies and achieve desirable optical and catalytic properties. We are also planning to extend the structural evolution to figure out the origin of chirality in nanoscale.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Symposium : **KCS1-7**
[KAIST-SRC Symposium] Frontiers in Multiscale Chirality
Room 101 WED 15:50
Chair: Myungeun Seo (KAIST)

Supramolecular Polymers Based on C3-Symmetric Triphenylene Triimides: From Point Chirality to Helicity

Byeong-Su Kim

Department of Chemistry, Yonsei University, Korea

A new type of C3-symmetric triphenylene triimides (TTI) bearing chiral oligo(ethylene glycol) side chains via imide linkages are developed in this study. By exploiting this unique TTI molecule as a building block, a supramolecular polymerization is explored on the basis of π-π stacking and hydrophilic/hydrophobic interaction depending on the type of solvents, rates of heating/cooling process, and the ratio of chiral-to-achiral TTI molecules, leading to thermodynamic aggregates. Most interestingly, the molecular point chirality of TTI monomer triggers the formation of a preferential helicity in fibrous structures as evidenced by a collection of spectroscopic analyses including UV/vis, PL, and CD together with AFM and TEM. In addition, the chirality of the resulting helical polymers is found to be modulated by irradiation with circularly polarized light.

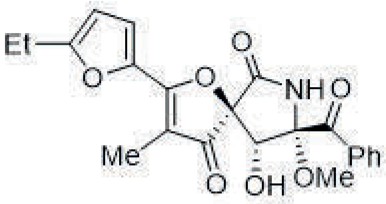
Symposium : **KCS1-8**
[KAIST-SRC Symposium] Frontiers in Multiscale Chirality
Room 101 WED 16:10
Chair: Myungeun Seo (KAIST)

Multiscale Chiral Architectures: A Molecular Level Approach

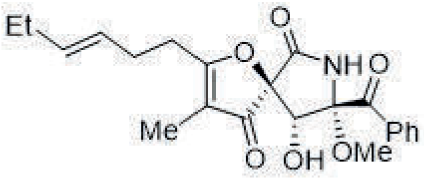
Sunkyu Han

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

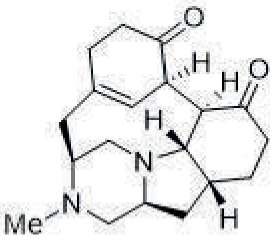
The Center for Multiscale Chiral Architectures (CMCA) aims to discover novel strategies and tactics for the synthesis, mechanistic understanding, and application of chiral architectures in various levels ranging from molecular to nanometer and macroscopic levels. As a member of CMCA, my research group, in collaboration with other center’s members, has been working on the understandings of chirality transfer and amplification at a molecular level. In this presentation, our progresses on CMCA-based researches on natural products will be presented. Molecular level chirality transfer and amplification will be discussed in the context of FD-838 and cephalimysin A synthesis.[1] Collaborative research efforts will be discussed by describing our synthetic efforts toward herquline A.[2] Our multiscale collaborative research will be introduced in the realm of synthesis and application of catechin derivatives. 1.Jo, D.; Han, S. "Total Synthesis of (–)-FD-838 and (–)-Cephalimysin A" Org. Lett. 2019, 21, 6045.2.Kim, T. T.; Lee, C.; Lee, H.-S.; Han, S. “Synthesis of the Pentacyclic Core of Herquline A” in preparation.



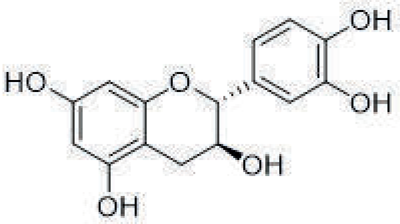
FD-838



cephalimysin A



herquline A



catechin

Symposium : **KCS2-1**

[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences

Room 102 WED 13:30

Chair: Yoonsoo Pang (GIST)

Molecular reaction dynamics in excited state by measuring nuclear wave packets

Taiha Joo

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

For a photochemical reaction occurring in an electronic excited state, several adiabatic and non-adiabatic processes are involved including vibrational relaxation, intramolecular vibrational energy redistribution (IVR), internal conversion, intersystem crossing, and curve crossing (via conical intersection). On experimental side, one powerful way to study the molecular reaction dynamics in excited states is to record the nuclear wave packet motions following the photoexcitation to the Franck-Condon state. Evolution of the vibrational wave packets can, in principle, provide potential energy surfaces (PES) through mapping of the PES of the excited state to the PES of the state that the molecule emits to, which is the ground state in most cases. Time-resolved fluorescence is a viable method to carry out such task. On theory side, non-adiabatic molecular dynamics simulation is an invaluable tool to unravel the detailed picture of the molecular reaction dynamics in the excited state. Recent progress on experimental advances towards this direction will be presented.

Symposium : **KCS2-2**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 13:40
Chair: Yoonsoo Pang (GIST)

Direct observation of the ultrafast structural dynamics engineering the fate of the excimer state

Dongho Kim

Department of Chemistry, Yonsei University, Korea

In π-conjugated organic photovoltaic devices, an excimer state has been generally regarded as a trap state which hinders the efficient excitation energy transport. However, it has been reported that the excimer often acts as an intermediate, which evolves into the charge separated state or multiexcitonic triplet pair state, suggesting the potential of the excimer state for application in desirable devices. Although it is clear that the structural dynamics in the excited state is crucial for the further evolution of the excimer state, tracking the structural change has remained unexplored. Here, we present the full structural dynamics of the excimer state using the ultrafast time-domain Raman spectroscopies. First, we directly probed the ultrafast structural evolution accompanying the excimer formation starting from the Franck Condon region, which further evolves into a relaxed excimer state along the intermolecular as well as solvation coordinates. Second, our results based on excited-state Raman measurements revealed that the ring deformation mode, which is tunable through the structural distortion, acts a crucial role in the control of excimer characteristics. This work showcases the ultrafast structural dynamics necessary for the excimer formation and control of excimer characteristics but also provides new criteria for designing the π-conjugated organic molecules to control the excited-state dynamics.

Symposium : **KCS2-3**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 13:50
Chair: Yoonsoo Pang (GIST)

MRSF as A Method of Choice for Nonadiabatic Molecular Dynamics (NAMD)

Cheol Ho Choi

Department of Chemistry, Kyungpook National University, Korea

It has been shown that a significant part of controversies regarding excited state dynamics can be attributed to the deficiency of CASSCF as well as popular TDDFT. To be a reliable methodology, a method should: (i) provide for a balanced and accurate account of the dynamic correlation as well as the multi-reference characteristics (including important double excitations) of the electronic states, (ii) be capable of correctly describing the conical intersections between the ground and excited electronic states, and (iii) be efficient enough to perform statistical dynamical sampling for several picosecondsThe recently developed mixed-reference spin-flip time-dependent density functional theory (MRSF-TDDFT; MRSF, for brevity) method, can become a good alternative, which enables fast and accurate computation of the ground and excited electronic states with the inclusion of the dynamic correlation and the multi-reference characteristics. An important advantage of MRSF before the usual LR-TDDFT is that MRSF enables proper computation of the S_1/S_0 conical intersections; which are crucial for the accurate description of the dynamics of the excited states, without the spin-contamination pitfalls of SF-TDDFT.

Symposium : **KCS2-4**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 14:00
Chair: Yoonsoo Pang (GIST)

Intramolecular Charge Transfer in the Excited States

Yoonsoo Pang

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

Intramolecular charge transfers (ICTs) of push-pull emitters between the electron donor and accepting groups connected by π-conjugated backbones are of great interest in the applications of solar cells, artificial photosynthesis, etc. The structural changes of chromophores during the ICT have long been investigated experimentally and theoretically. However, the structures in the ICT states, such as the "twisted" or "planar" geometry of electron donor or acceptor groups proposed in many theoretical studies, have not been verified experimentally via time-resolved vibrational spectroscopy. In this work, femtosecond stimulated Raman spectroscopy (FSRS) with both high temporal ($^{-1}$) are used investigate the structural changes upon the ICT of push-pull emitters with the nitro group as the electron acceptor, 4-dimethylamino-4′-nitrobiphenyl (DNBP) and 4-dimethylamino-4′-nitrostilbene (DNS). Twist of the electron-donating or accepting group leads to the changes in the skeletal stretchings of two phenyls (ν_{8a}) and central ethylene ($\nu_{C=C}$; DNS only). The potential surface of DNS toward the ICT state appears strongly coupled to low-frequency vibrational modes of in-plane and out-of-plane deformations leading to the rotation of electron donor or acceptor group. The coherent oscillations resulting from the anharmonic coupling of the potential surfaces are observed in the skeletal vibrational modes of DNS. These coherent oscillations are absent in the ICT of DNBP, which is suggested to occur via a barrier-less potential surface by many theoretical studies.

Symposium : **KCS2-5**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 14:30
Chair: Sung Jee Kim (POSTECH)

Coherent Emission from Nanoparticles

Sung Jee Kim

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

An ensemble of emitters can behave very differently from each individual constituents when they interact coherently with a common light field. After excitation of such an ensemble, collective coupling can give rise to a many-body quantum phenomena. An intense bursts of light, also known as superfluorescence, can be observed. This phenomenon requires a fine balance of interactions between the emitters and their decoupling from the environment. So far, such superfluorescence has been observed only for a limited number of systems especially for colloidal nanoparticle systems. The generation of superfluorescent light in colloidal nanocrystals may suite for next-generation photonic or optoelectronic sources that have been unattained by inhomogeneous emission broadening, low oscillator strength, fast exciton dephasing, etc. Here, we discuss coherent emissions from nanoparticle systems. These mesoscopically extended coherent states could be potentially also used for entangled multi-photon quantum light sources.

Symposium : **KCS2-6**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 14:40
Chair: Sung Jee Kim (POSTECH)

The Intra-band electron dynamics of HgS Quantum dot Studied by Infrared Pump-Probe and 2D-IR Spectroscopy

Kyungwon Kwak

Department of Chemistry, Korea University, Korea

Quantum dots absorbing mid-infrared light have been synthesized and tested as a potential candidate for the promising materials for mid-IR detection. Intra-band transition is induced by the absorption of infrared photon. Electronic excited state induced by infrared field shows fast relaxation dynamics due to the strong electron-phonon coupling. The relaxation time show two characteristic relaxation times; fast one is size-independent and the other shows frequency dependence due to the structural inhomogeneity. The HgS Collidal Quantum Dots (CQDs) with Mid-IR intraband gap can be fascinating materials for IR photodevices. Here, we reported the interesting relaxation dynamics of Dodecanethiol-doped HgS CQDs which have size-dependent intraband gap. By using IR pump-probe techniques, we observed pump power-independent fast decaying dynamics (1.2 ± 0.1 ps) accelerated by Auger process in CQDs with biexciton generation and slow decay process (>300 ps) caused by Phonon bottleneck for CQDs with single photon absorption. Moreover, the intermediate component (~20 ps) is also observed and assigned to the interband relaxation process. Surprisingly, we found that the Auger relaxation process, frequently observed through the bandgap transition under high photoexcitation energy, also occurs through intraband transitions in the CB. In conjunction with Ab-initio calculation, it was also revealed that the intraband transition is efficiently coupled with the nanocrystal surface, which successfully explains the physical phenomena such as phase transition from the intraband transition to the localized surface plasmon resonance (LSPR) of nanocrystals through increasing the carrier density, or the high surface sensitivity of the self-doped quantum dot.

Symposium : **KCS2-7**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 14:50
Chair: Sung Jee Kim (POSTECH)

Temperature evolution of electronic coherence in solid

Ji Hoon Shim

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

The temperature-dependent evolution of the Kondo lattice is a long-standing topic of theoretical and experimental investigation and yet it lacks a truly microscopic description of the relation of the basic f-d hybridization processes to the fundamental temperature scales of Kondo screening and Fermi-liquid lattice coherence. In this talk, the temperature-dependence of f-d hybridized band dispersions and Fermi-energy f spectral weight in the Kondo lattice system CeCoIn5 is investigated using first principles dynamical mean field theory (DMFT) calculations containing full realism of crystalline electric field states. All the calculated results are directly compared to f-resonant angle-resolved photoemission (ARPES). Our results reveal f participation in the Fermi surface at temperatures much higher than the lattice coherence temperature, T*≈ 45 K, commonly believed to be the onset for such behavior. The identification of a T-dependent crystalline electric field will be discussed with its contribution to T* as well as local Kondo temperature TK.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Symposium : **KCS2-8**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 15:00
Chair: Sung Jee Kim (POSTECH)

Cluster Frameworks

Sarah Sunah Park

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

The hierarchical assembly of the colloidal nanocrystals is powerful approach to bottom-up construction of functional materials and this has been extensively explored. However, since nanocrystals are difficult to precisely control at atomic levels due to polydispersity and complex surface chemistry, assembly approaches, using molecular clusters as superatomic building blocks, is an attractive alternative. Owing to their diverse composition with redox activity, large magnetic moments, and luminescence, metal clusters relying on electrostatic interaction are regarded as powerful tools for the construction of tunable materials which have shown remarkable properties in electronic and thermal transport. In this presentation, new strategy for assembling and utilizing the cluster frameworks will be discussed.

Symposium : **KCS2-9**

[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences

Room 102 WED 15:30

Chair: Young Min Rhee (KAIST)

Vibrational Coherence and Molecular Dynamics

Young Min Rhee

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

Flourescence through the conversion from the lowest triplet state to the lowest singlet is an important mechanism for efficiently generating light emitting state of organic molecules. A second-order perturbation effect mediated by an upper triplet or singlet may engage importantly for the process, and whether the mediation happens in a superexchange manner is still debatable. Here, we will show that the superexchange effect manifests in a peculiar way for a multiple resonance emitter. When the spin-orbit coupling becomes negligible due to the strong pi-pi* transition character as in a rigid single-domain emitter, superexchange starts to participate importantly. Indeed, the superexchange appear to utilize the coherent superposition between multiple triplet states for enhancing spin cross-over. Other details such as the participation of vibrational states are also compared.

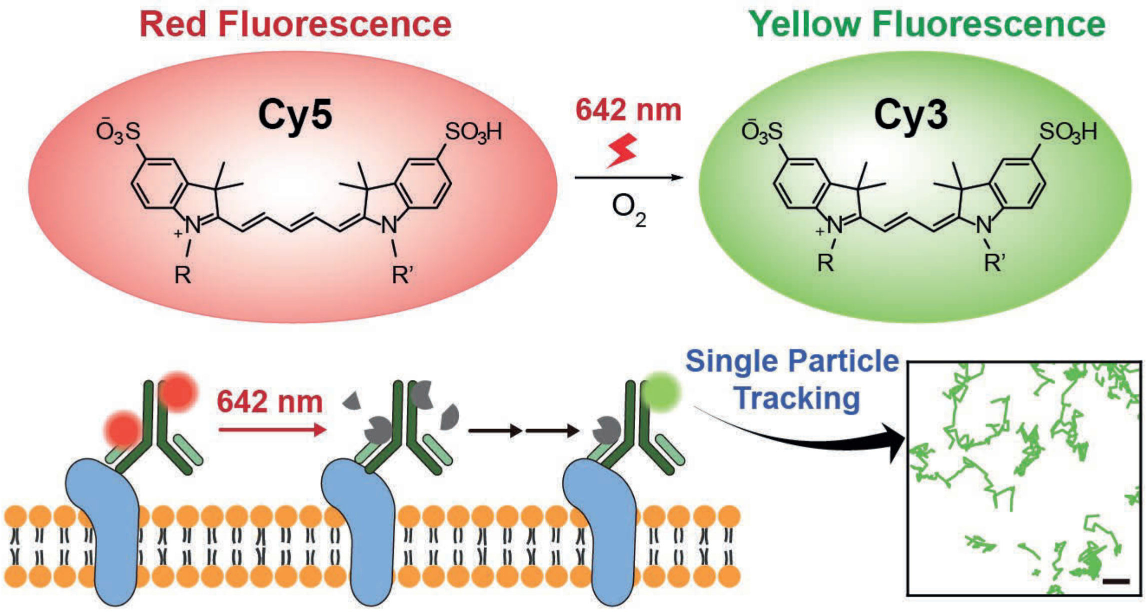
Symposium : **KCS2-10**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 15:40
Chair: Young Min Rhee (KAIST)

New method for single-protein tracking in a living cell using photoconversion

Nam Ki Lee

Division of Chemistry, Seoul National University, Korea

Recent advances in single-molecule fluorescence microscope techniques have allowed single-molecule sensitivity to probe various protein-DNA interactions, their structural changes, and fundamental cellular processes in a living cell. Here, I present our recent progress in developing new methods for single-protein tracking and observing protein movement in living cells. We directly observe the dynamics of transcription and the movement of the subcellular localization of genes actively transcribed by RNAP in living cells at the sub-diffraction limit resolution. We also proved new photophysical properties of Cyanine dyes, i.e., photoconversion to blue-shifted products. Using this new property, we developed a new method for single-protein tracking in a living cell without using additive agents and UV illumination.


Red Fluorescence
Cy5
$^{-}O_3S$
SO_3H
N
R
R'
642 nm
O_2
Yellow Fluorescence
Cy3
$^{-}O_3S$
SO_3H
N
R
R'
642 nm
Single Particle Tracking

Symposium : **KCS2-11**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 15:50
Chair: Young Min Rhee (KAIST)

Exciton-driven ionization for the mass spectrometric analysis of semiconductor nanoparticles

Jongcheol Seo

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

The efficient ionization is of importance for characterizing semiconductor nanoparticles (quantum dots, QDs) using mass spectrometry. The most widely used is matrix-assisted laser desorption/ionization (MALDI) which typically uses a UV laser. The matrix molecules are often excited and even ionized by the ejection of an electron to yield radical cation which may further take an electron from neutral QDs to generate QD radical cation. Here, UV laser irradiation not only produce matrix radical ions but also able to directly excite QDs to yield electron-hole pairs, excitons. Therefore, the dissociation of an exciton into a free electron and a hole, and the efficient extraction of an electron is critical to generate QD ions. To accomplish that, we try to control electron behavior in the UV-excited QDs. Firstly, we implement efficient electron acceptor as a matrix molecule. Secondly, we try to suppress the electron-hole recombination and thus, increase electron transfer probability. Representatively, using an electron-deficient fluorinated porphyrin as a matrix molecule has shown great enhancement in QD MALDI-MS signal compared to the other conventional matrix molecules. Applying quenching QD photoluminescence by applying Cu-doping also shows the increase of QD ionization efficiency. Understanding the details in the photoexcitation and the exciton dynamics of QDs will further benefit this research, and therefore active collaborations in the center is necessary.

Symposium : **KCS2-12**
[POSTECH-SRC Symposium] Measurements and Theory of Electronic and Nuclear Quantum Coherences
Room 102 WED 16:00
Chair: Young Min Rhee (KAIST)

X-ray Studies of Water's Anomalous Properties and the Mechanism of Chemical Reactions

Kyung Hwan Kim

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

X-ray science has evolved dramatically with the use of X-ray free electron lasers (XFELs) that can generate ultrashort X-ray pulses with unprecedented brilliance and coherence. This has been a breakthrough for many X-ray related techniques on a broad range of scientific disciplines and brought us to investigate many interesting new sciences that was previously not accessible. In this talk, our recent X-ray studies of the origin of anomalous properties of water [1-2] and ultrafast reaction dynamics with free electron laser facilities will be shown.In the liquid form, water has numerous anomalous properties as compared to other liquids such as density maximum at 4-degree C. As an explanation for these anomalous experimental observations, a hypothetical liquid-liquid transition (LLT) and a liquid-liquid critical point (LLCP) has been proposed but has never been proved experimentally. Recently, we developed a new experimental technique utilizing FELs and found the first [1] and second [2] experimental evidence of the existence of the Widom line which is supposed to emanate from the LLCP.Reference[1] K. H. Kim et al., "Experimental Observation of the Liquid-Liquid Transition in Supercooled Water", Science, 370, 978-982 (2020).[2] K. H. Kim et al., "Liquid-Liquid Phase Separation in Supercooled Water from Ultrafast Heating of Low Density Amorphous Ice", manuscript in preparation.

Symposium : **KCS3-1**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 13:30

Chair: Wonwoo Nam (Ewha Woman University)

Molecular Functional Models of Photosynthesis

Shunichi Fukuzumi

Graduate School of Science and Engineering, Meijo University, Japan

Artificial photosynthesis is urgently required in order to solve global energy and environmental issues. This lecture focuses on the past and future of artificial photosynthesis. Artificial photosynthesis consists of five units: the light–harvesting (LH) unit, the charge–separation (CS) unit, the catalytic unit for water reduction, the catalytic unit for water oxidation, and the catalytic CO2 fixation unit. We have developed a variety of photosynthetic reaction center models composed of organic electron donors and acceptors linked by covalent or non-covalent bonding, which undergo efficient charge separation and slow charge recombination. The efficient charge-separation step has been successfully combined with the catalytic water reduction step with earth-abundant metal catalysts to develop efficient photocatalytic hydrogen evolution and CO2 reduction systems. The photocatalytic oxidation of water with O2 in the air to produce H2O2 has been achieved, together with the development of one-compartment H2O2 fuel cells. The first functional mimic of photosystem II (PSII) is also reported together with the combination with a PSI mimic.

Symposium : **KCS3-2**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 14:35

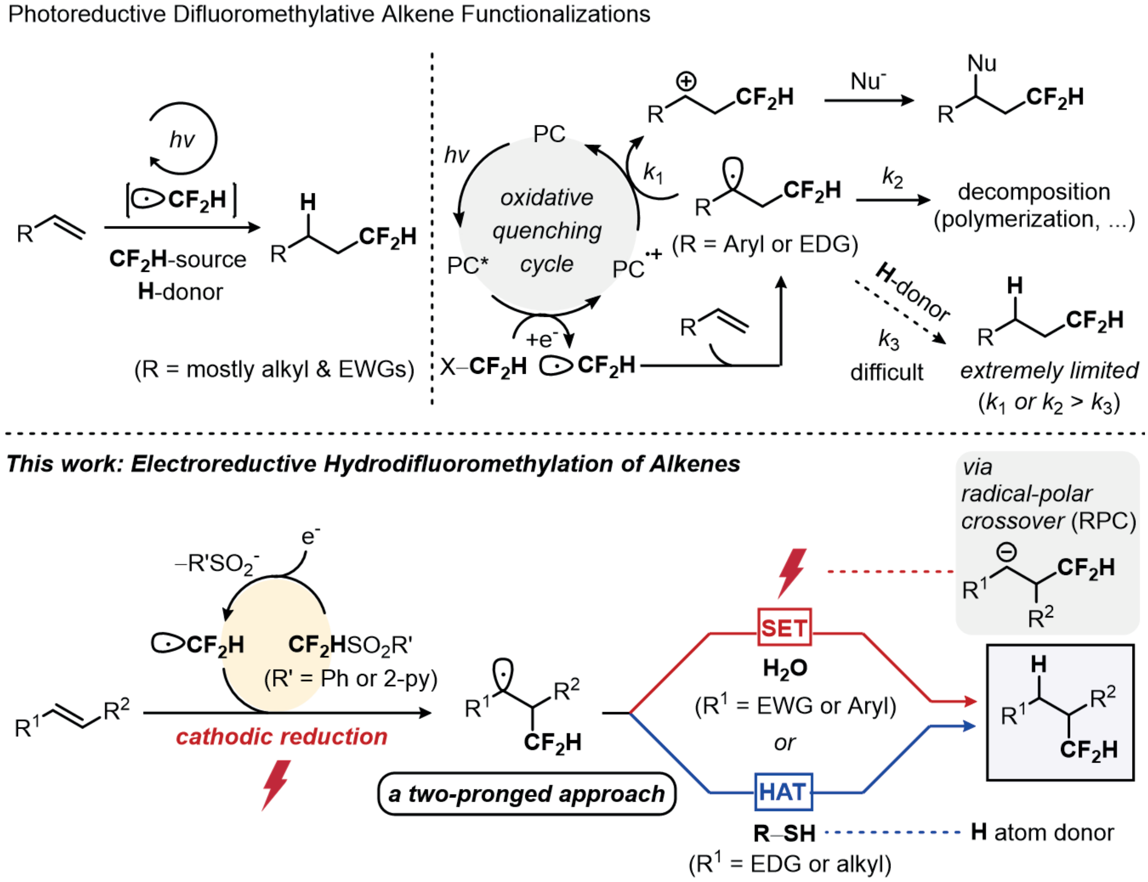
Chair: Nak Cheon Jeong (DGIST)

Radical hydrodifluoromethylation of alkenes via an electroreductively triggered two-pronged approach: the key distinction between organic photosynthesis and electrosynthesis

Hyunwoo Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Despite their importance in pharmaceutical applications, synthetic routes to difluoromethylated pharmacophores are still very limited. To this end, we have devised a two-pronged strategy that enables hydrodifluoromethylation of a wide range of alkenes by means of reductive radical-polar crossover or direct hydrogen atom transfer from electroreductively generated carbon-centered radical intermediates. The newly developed strategy is generally valid to a wide range of alkenes and grant access to a late-stage modification of pharmacophores.



Photoreductive Difluoromethylative Alkene Functionalizations

This work: Electroreductive Hydrodifluoromethylation of Alkenes

- Hydrodifluoromethylation of both unactivated & activated alkenes
- CF_2H source choice upon the electronic properties of the employed substrates
- Late-stage functionalizations with commercially available radical CF_2H sources
- Inexpensive H_2O or PhSH as the hydrogen sources

Symposium : **KCS3-3**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 14:50

Chair: Nak Cheon Jeong (DGIST)

Light-Induced Switching of Block Copolymer Particle Structure and Property

Hongseok Yun

Department of Chemistry, Hanyang University, Korea

In this talk, I will present the light-driven structural reorganization of block copolymer (BCP) particles. The key strategy is the design of azobenzene-grafted Au nanoparticles (Au@Azo NPs) as photo-responsive surfactants by taking advantage of the photoisomerization of azobenzene ligands. Visible light resulted in the formation of onion-like spherical polystyrene-block-poly(2-vinylpyridine) (PS-b-P2VP) BCP particles due to the presence of non-polar trans-Azo ligands, while the UV-driven isomerization into polar cis-Azo isomers induced the transformation of the spheres to ellipsoids by forming a relatively neutral BCP-surrounding interface. The shape evolution process was investigated using a cryogenic electron microscope, showing the selective rearrangement of Au@Azo NPs on each domain of the BCP particle surface. Finally, the light-controlled optical behavior of these hybrid BCP particles was successfully demonstrated by achieving shape-dependent energy transfer between fluorescent dyes and Au NPs, translating the change in particle shape into an optical signal.

Symposium : **KCS3-4**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 15:05

Chair: Nak Cheon Jeong (DGIST)

Turning Photons into Chemical Reactions: Kinetic Studies of Plasmonic Au Photocatalysts

Youngsoo Kim

Department of Chemistry, Yeungnam University, Korea

Plasmonic noble metal nanoparticles have recently received increased attention as visible-light photocatalysts. Heterostructured plasmonic photocatalysts are composed of semiconductor and noble metal nanoparticles, i.e., Au/ZnO, Au/TiO_2, and have been shown to drive important chemical reactions like CO_2 reduction or water splitting via absorption of visible light. In such a system, however, the mechanisms for photoexcited carrier harvesting and migration have not been clearly elucidated as these mechanisms compete with rapid energy relaxation within the metal. And the role of plasmonic nanoparticles has been limited as a light-absorbing antenna. We accomplished a simple one-electron photochemical reaction using plasmonically excited Au nanoparticles in the absence of any supporting semiconductor for better mechanistic insight. In this talk, we will comprehensively deal with the kinetic study of the photochemical reaction, the changing in activation energy by light contribution, and the nature of hot electron transfer in a donor-bridge-acceptor system on Au catalyzed photochemical reaction in detail.

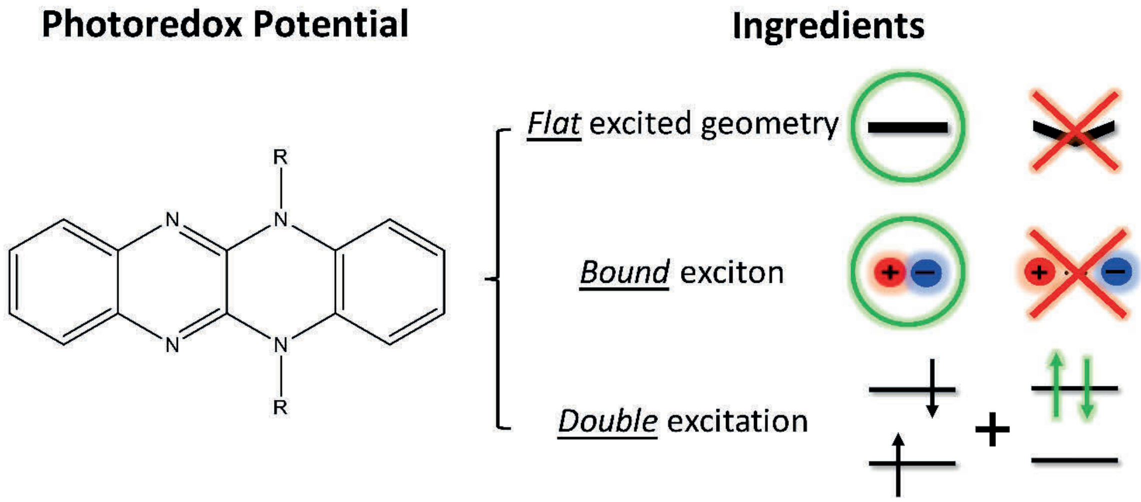
Symposium : **KCS3-5**
[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges
Room 103 WED 15:20
Chair: Nak Cheon Jeong (DGIST)

Spin-Flip Density Functional Theory for Redox Properties of Organic Photoredox Catalysts in Excited States

Hyungjun Kim

Department of Chemistry, Incheon National University, Korea

Photoredox catalysts (PCs) have contributed to the advancement of organic chemistry by accelerating conventional reactions and enabling new pathways through the use of reactive electrons in excited states. Instead of labor-intensive manual experimentation, quantum chemical simulations could explore the enormous chemical space more efficiently. The reliability and accuracy of quantum chemical simulations have become important factors for material screening. We designed a theoretical protocol capable of predicting redox properties in excited states with high accuracy for a selected model system of dihydroquinoxalino[2,3-b]quinoxaline derivatives. Herein, three factors were considered as critical to achieving reliable predictions with accurate physics: the solvent medium effect on excited-state geometries, an adequate amount of Hartree–Fock exchange (HFX), and the consideration of double-excitation character in excited states. We established a theoretical protocol that could provide highly accurate estimations of photophysical properties and ground-/excited-state redox properties, focusing on the three factors mentioned above. Geometry optimization with DFT and TDDFT employing the B3LYP functional (20% HFX) in solution and energy refinement by SF-DFT reproduced the experimental redox properties in the excited and ground states remarkably well with mean signed deviations (MSDs) of 0.01 and −0.15 V, respectively. This theoretical protocol is expected to contribute to the understanding of exciton behavior in organic PCs and to the efficient design of new promising PC candidates.


Photoredox Potential
Ingredients
R
N
N
N
N
R
Flat excited geometry
Bound exciton
+
−
Double excitation
+

Symposium : **KCS3-6**
[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges
Room 103 WED 15:35
Chair: Nak Cheon Jeong (DGIST)

Functional Integration of Catalysts for Efficient Utilization of Photogenerated Charge Carriers

Sung Yul Lim

Department of Chemistry, Kyung Hee University, Korea

Photoelectrochemical cell (PEC) renders a promising route to produce chemical fuels with lower electrical energy input, aided by photogenerated charge carriers in semiconductors. For commercialization of PEC, improving photoelectrochemical efficiencies is crucial while lowering the materials and fabrication costs. In this regard, optimization of semiconductor/catalyst interface is required to achieve efficient light absorption in semiconductor materials, large potential gradient at the interface, and high catalytic activity of catalytic materials. Herein, photoelectrochemical effect of physical and chemical control of catalysts on the semiconductor surface will be discussed, which leads to efficient management of light-semiconductor interaction and electron transfer to chemical reactant. The spatial control of catalysts can minimize parasitic light absorption/scattering by the catalytic layers. Moreover, this spatial control of catalysts possibly provokes synergistic mechanistic interaction between the catalysts and exposed semiconductor surface to electrolyte. The proper chemical compositions of catalysts can induce large potential gradient at the semiconductor/catalyst junction for efficient electron transport while enable the proficient electron transfer events. The discussion through this presentation can contribute to design better semiconductor/catalyst interface for commercialized PEC.

Symposium : **KCS3-7**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 15:55

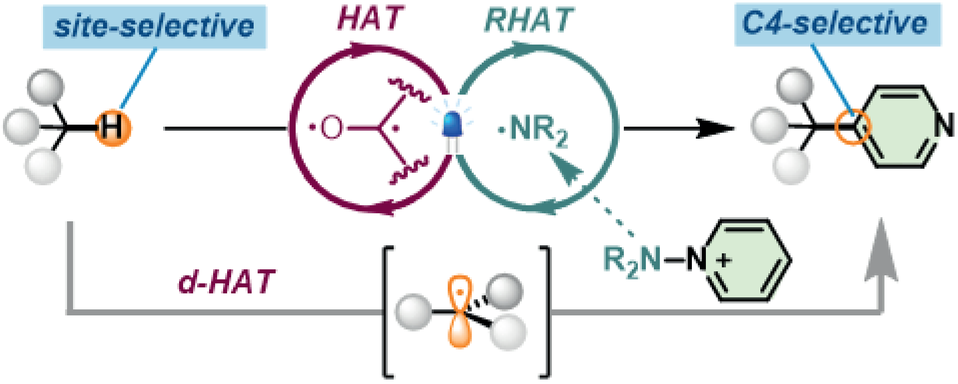
Chair: Mi Hee Lim (KAIST)

Site-Selective Direct C–H Pyridylation of Unactivated Alkanes *via* Photocatalysis

Wooseok Lee, Sungwoo Hong*

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

As interest in environmental issues increases, efforts are being made to develop eco-friendly reactions that do not produce industrial waste in the field of organic chemical synthesis. Reaction development using visible light is also in the spotlight in the field of organic synthesis. Various reactions using light have been reported exponentially, and the efficiency of the reaction is increasing through the development of new photocatalysts, light sources, and photoreactors.Site-selective functionalization of $C(sp^3)$-H bonds using visible light is a challenging and useful reaction in the broad field of chemical research. In this presentation, we describe a new synthetic route for the site-selective C–H pyridylation of unactivated hydrocarbons via direct Hydrogen Atom Transfer(d-HAT) catalyst and reverse hydrogen atom transfer(RHAT) reagent. The selective pyridylation of more substituted, electron-rich C–H bonds in abundant chemical feedstocks was achieved by N-aminopyridinium salts. We provide a new catalytic system for the direct construction of valuable compounds under ambient reaction conditions. Moreover, this method is a powerful tool that enables functionalization in a wide range of fields from general alkane feedstocks under mild, metal-free reaction conditions.


site-selective
HAT
RHAT
C4-selective
H
•O
•NR$_2$
N
R$_2$N–N+
d-HAT

Symposium : **KCS3-8**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 16:05

Chair: Mi Hee Lim (KAIST)

Development of highly efficient and stable perovskite solar cells

Kyoungwon Choi, **Taiho Park**[1,*]

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

Perovskite solar cells (PSCs) have attracted tremendous attention due to their excellent optical and electrical properties. With intense research efforts on PSCs, the power conversion efficiency has been dramatically improved from 3.8% to over 25%. However, the instability of PSCs under external stresses (e.g., humidity, light, and heat) hampers their practical use. Therefore, many studies have been conducted to solve these instability issues and demonstrated that the UV light and humidity instability can be alleviated by using dopant-free polymer, encapsulation, and UV light filter, but thermal stability cannot be secured. The low thermal stability of perovskite is mainly caused by complex factors of heat generated inside the device, electron-transporting layer, hole-transporting layer, and perovskite layer. In this point of view, we must consider all factors holistically rather than individually and further studies are needed to achieve thermally stable PSCs. Here, we systematically investigated the effect of each factor on the reduction of device performances and tried to realize highly efficient and stable PSCs by developing novel strategies.

Symposium : **KCS3-9**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 16:15

Chair: Mi Hee Lim (KAIST)

Emergence, Amplification, and Suppression of Supramolecular Chirality by Circularly Polarized Light

Jun Su Kang, Woo youn Kim[1,*], Myungeun Seo[*]

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

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

Homochirality in nature is speculated as a result of transfer and amplification of a small amount of primal chiral bias from molecular scale to mesoscopic and macroscopic scales. Circularly polarized light (CPL) has been considered as a possible origin of the homochiral environment by transferring chiral information to molecular matter. Here, we report emergence of supramolecular chirality via CPL-induced supramolecular co-polymerization of chiral and achiral triphenylamine (TPA) derivatives. We will show competition between molecular chirality and CPL by varying compositions of chiral TPA units. The results of overwriting and amplifying molecular chirality by CPL will be provided to compare contributions of two stimuli to supramolecular helices in a quantitative manner.

Symposium : **KCS3-10**
[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges
Room 103 WED 16:25
Chair: Mi Hee Lim (KAIST)

Mid-Infrared Energy State Study in Self-Doped Quantum Dots

Dongsun Choi, Kwang Seob Jeong*

Department of Chemistry, Korea University, Korea

Natural high carrier concentration and electron occupancy in the conduction band are remarkable properties of self-doped colloidal quantum dots (CQDs). It has been revealed that the self-doping property promotes the intraband transition but forbids the interband transition of the material. Among those self-doped CQDs, the silver chalcogenides CQDs have been vigorously studied recently due to the non-toxic nature of the silver. Furthermore, the silver chalcogenides CQDs show a quantum-plasmonic effect, suggesting the next quantum jump in the self-doping CQDs study. The Ag_2Se CQDs is a fascinating MWIR active material that has a high potential for future application. The Ag_2Se CQDs intraband transition is reported for the first time by Prof. Jeong's group in ACS photonics. A spectro-electro-chemistry (SEC) method has disclosed the intraband transition of Ag_2Se CQDs and proves that the interband transition of Ag_2Se CQDs exists at higher energy. Interestingly, the silver selenide CQDs have revealed a broken degeneracy of the p-state. The Ag_2Se CQDs undergo the crystal structural transformation from cubic to tetragonal nanocrystal structure with increasing size. Accordingly, the corresponding degeneracy broken of the 1Pe states is optically observed along with the structural transformation. Strikingly, the Ag_2Se CQDs plasmonic character coexists with the steady-state intraband electronic transition, which indicates the quantum-plasmon characters in the self-doped Ag_2Se CQDs. The intraband transition study could elucidate the challenging observations such as blinking of QDs, excessive charging in QDs device, and hot electron dynamics in conduction band coupled to nanocrystals' surface states.

Symposium : **KCS3-11**
[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges
Room 103 WED 16:35
Chair: Mi Hee Lim (KAIST)

Probing the structural dynamics controlling the nature of the exciton by time-domain Raman spectroscopy

Yongseok Hong, Dongho Kim[*]

Department of Chemistry, Yonsei University, Korea

Since the intermolecular interactions are hyper-sensitive to molecular packing structures, it has been suggested that morphological control is crucial for inducing the excimer (Ex) or multiexcitonic (ME) intermediate states. However, it is difficult to generalize the molecular design for the desirable photovoltaic devices through synthetic approaches considering the complexity of the excited state. Due to the difficulties, the direct observation of the ultrafast structural dynamics manipulating the nature of the exciton state has remained elusive so far. Here, we present the direct observation of the full structural dynamics of the Ex and ME states in two PBI dimers using TR-ISRS.The TR-ISRS results provide important insights. Firstly, the out-of-plane mode is a key vibration to trigger the excimer formation. We suggest that the most important structural parameter in the excimer formation is the intermolecular distance along with the stacking axis. Second, the singlet fission process is accompanied by the distinct appearance of the sliding mode, which manifests the importance of charge-transfer interaction to evoke the multiexcitonic state in PBIs. In conclusion, our observations not only help the researchers in the field clarify the fundamental information on the structural dynamics of the exciton state but also present the guidelines for designing the π-conjugated organic chromophores of the PBI family and beyond for application in OPV devices.

Symposium : **KCS3-12**
[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges
Room 103 WED 16:45
Chair: Mi Hee Lim (KAIST)

Theoretical insights into the potential-dependent competition between electrocatalytic dinitrogen reduction and hydrogen evolution reactions

Changhyeok Choi, Geun Ho Gu, Yousung Jung*

Department of chemical and biomolecular engineering, Korea Advanced Institute of Science and Technology, Korea

The electrochemical N_2 reduction reaction (NRR) produces ammonia cleanly and sustainably at ambient conditions. Various catalysts have demonstrated NRR activity at room temperatures, but the yield rate and the faradaic efficiency (< 10 %) are too low for the economic production, due to unwanted side reactions known as hydrogen evolution reaction (HER). More quantitatively, potential-dependent measurements often showed that the NRR activity begins to decrease at low overpotential region. The maximum NRR activity has been generally observed at insignificant overpotential, leading to the NRR current density much smaller than the expected mass-transfer-limited values. While the HER has been suggested to be responsible for this phenomenon, the mechanistic origin has not been clearly explained. In this talk, we discuss the potential-dependent competition between NRR and HER based on the kinetics and active site coverages. [1] We used density functional theory calculations conjunction with the constant electrode potential model and microkinetic modeling. Our potential-dependent simulation agrees with the experimentally observed trend. We find that the H coverage and N_2 coverage crossover leads to the premature decrease of NRR activity. The crossover originates from the larger charge transfer in H^+ adsorption than N_2 adsorption. This crossover is a general phenomenon seen in various heterogeneous catalysts, posing a fundamental challenge to realize practical electrochemical NRR. We suggest several strategies to overcome the challenge based on the present understandings.

[1] C. Choi, et al. Nat. Commun. 2021, 12, 4353

Symposium : **KCS3-13**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 16:55

Chair: Mi Hee Lim (KAIST)

Size-Dependent Light Harvesting from Nonthermalized Excited States of Gold Clusters

SangMyeong Han, Hongmei Xu, Dongil Lee[*]

Department of Chemistry, Yonsei University, Korea

Light harvesting is central to many photonic materials. The light harvesting efficiency in these materials is, however, generally reduced because upper excited-state energy is lost by energy-dissipating internal conversion (IC) and vibrational relaxation processes. Atomically precise gold clusters have emerged as a new class of materials because of their unique bulk-to-molecule transition characters, where discrete electronic states emerge and electronic band energetics lead to quantum confinement effects. Recently, the presence of relatively slow IC processes in the subpicosecond-to-picosecond range has been generally observed in molecule-like gold clusters. Herein, by conjugating energy acceptor aminofluorescein (AF) to the gold nanoclusters, new energy harvesting methodology via energy transfer from the nonthermalized state of gold nanoclusters, which was achieved by relatively slow IC process is demonstrated.

Steady-state photoluminescence measurements of AF-conjugated Au18, Au22, and Au25 clusters show notable AF emission upon high-energy excitation of gold clusters. Femtosecond transient absorption measurements reveal that the IC processes of Au18, Au22, and Au25 are relatively slow whereas IC processes of larger clusters overwhelm the energy transfer rate. Energy gap and spectral overlap have been considered to another descriptor for efficient nonthermalized energy transfer. Herein, a new avenue for energy harvesting from nonthermalized upper excited states of gold clusters, which would otherwise be lost as heat, is opened up.

Symposium : **KCS3-14**

[International Symposium for Emerging Investigators] Light-Matter Interaction and Electron Transfer: State of the Art and Remaining Challenges

Room 103 WED 17:05

Chair: Mi Hee Lim (KAIST)

Hydrogen Atom Transfer Coupled Dye-Sensitized Photoelectrochemical Cell for Oxidative Cleavage of Lignin

Hyeong Cheol Kang, Saerona Kim[1], Gyu Leem[1,*], Jae-Joon Lee[*]

Department of Energy and Materials Engineering, Dongguk University, Korea
[1]Chemistry, State University of New York, United States

As the decomposition process of lignin, there were several processes was reported. However, low selectivity of oxidize/cleavage is one of prime issues because of reaction under harsh condition like high temperature and high pressure. To overcome these problems, especially, dye-sensitized photo-electrochemical(HAT-DSPEC), which used photocatalyst(RuC) and heterogeneous catalysts incorporating system was suggested. And it represent conversion efficiencies over 90% under 24 h, light illumination (AM 1.5G). However, this kinds of Ruthenium based sensitizer has disadvantages like low stability, high cost and low adsorption coefficient. In this study, for highly stable HAT-DSPEC process, Ru based sensitizer was replaced by organic dye(5-[4-(diphenylamino)phenyl]thiophene-2-cyanoacrylic acid, L1) which has highly stable and molar adsorption coefficient. Also three kinds of organic nitroxyl mediators (HAT) was used such as 2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO), 4-Acetamido-TEMPO (ACT), 9-azabicyclo[3,3,1]nonan-3-one-9-oxyl (Keto-ABNO). Each HATs (TEMPO, ACT and keto-ABNO) showed different reactivity and conversion efficiency (about 60%, 65% and 90%). In HAT-ODSPEC(organic dye-sesitized photo-electrochemical cell), Keto-ABNO showed highest conversion efficiency with 2-ol(S,G). This HAT-ODSPEC process provides a unique foundation to perform selective C−C bond cleavage for real lignin conversion technologies.

Symposium : **KCS5-1**
Future Information Technology for 'Super-Connected' Creative Society [The 15th Story of Future IT Technology with Dongwoo Fine-chem Co., Ltd.]
Room 102 THU 15:50
Chair: Jongsoo Lee (DONGWOO FINECHEM)

Challenges in Wet Chemical Processes for Semiconductor Scaling Down

Sangwoo Lim

Department of Chemical and Biomolecular Engineering, , Yonsei University, Korea

As silicon-based semiconductor approaches the physical scaling down limit, various efforts have been made to solve the problems which arose with scaling down of devices. One method to solve the problems is to introduce 3D structures such as FinFET, gate-all-around and vertical-NAND into the device architectures. The other method is to introduce new materials to cope with the device scaling down and improve the performance. Although wet chemical processes in semiconductor manufacturing are somewhat conservative and their changes are not that rapid as compared to other processes such as photolithography, it is obvious that new technologies are needed in the wet chemical processes also. In this presentation, several wet chemical approaches to the current device manufacturing process are introduced. Removal of particles from the semiconductor surfaces, new drying technology to avoid pattern collapse and other key issues regarding current wet chemical processes are discussed. In particular, recent progress in selective Si_3N_4 etching, which is one of the most important and challenging wet chemical processes in the current semiconductor manufacturing business, is presented. Including reaction mechanism of Si_3N_4 etching in H_3PO_4, control of etching rate, selectivity and oxide regrowth will be discussed. In addition, efforts to make selective Si_3N_4 etching in non-H_3PO_4 based fluid will be presented.

Symposium : **KCS5-2**
Future Information Technology for 'Super-Connected' Creative Society [The 15th Story of Future IT Technology with Dongwoo Fine-chem Co., Ltd.]
Room 102 THU 16:30
Chair: Jongsoo Lee (DONGWOO FINECHEM)

EUV Lithography: Principles and Key Materials

Jinho Ahn

Department of Material Science and Engineering, Hanyang University, Korea

Extreme Ultra Violet lithography (EUVL) is the most advanced patterning technology which can be applied to the mass production of semiconductor devices. Due to the highly absorbing characteristics of EUV wavelength, EUVL is operated by reflective optics rather than by refractive optics. Due to the continuous efforts to solve the technical issues, EUV lithography began to be inserted into high volume manufacturing recently. It took more than 32 years to get ready for industrial application since the first pioneering studies on EUV lithography. The source power, which has been a bottleneck for a long time, showed more than 10x improvement during the last five years and now 250W is achieved in factory. There has been a great progress in mask blank defectivity but mask protection during lithography process may be necessary for the printable fall-on adder defects. EUV pellicle is now showing a lot of progress to meet the stringent requirements on the optical, mechanical, chemical and thermal properties. Resolution of photoresist is improving while we are struggling on the resist sensitivity and line width roughness (LWR). But it is good to know that EUV lithography is an extension of optical lithography. This means that most of the resolution enhancement technologies developed in DUV lithography can be applied in EUV lithography. Further extension of resolution limit is possible through high-NA system or further reduction of wavelength. During the presentation, some of important technical issues on the key materials in addition to the basic principles of EUV lithography will be introduced.

Symposium : **KCS5-3**
Future Information Technology for 'Super-Connected' Creative Society [The 15th Story of Future IT Technology with Dongwoo Fine-chem Co., Ltd.]
Room 102 THU 17:10
Chair: Jongsoo Lee (DONGWOO FINECHEM)

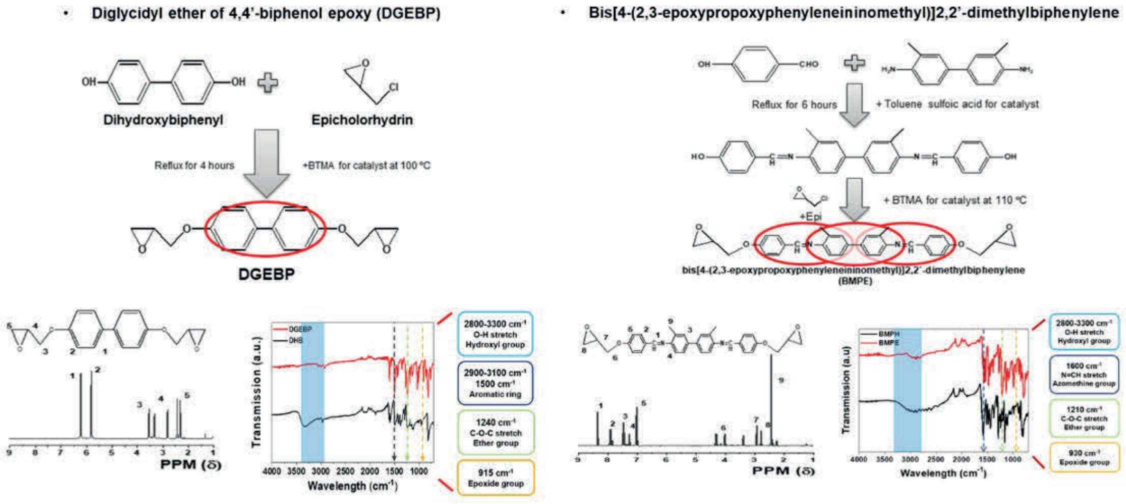
Rational design of epoxy molding compound for reliability and workability

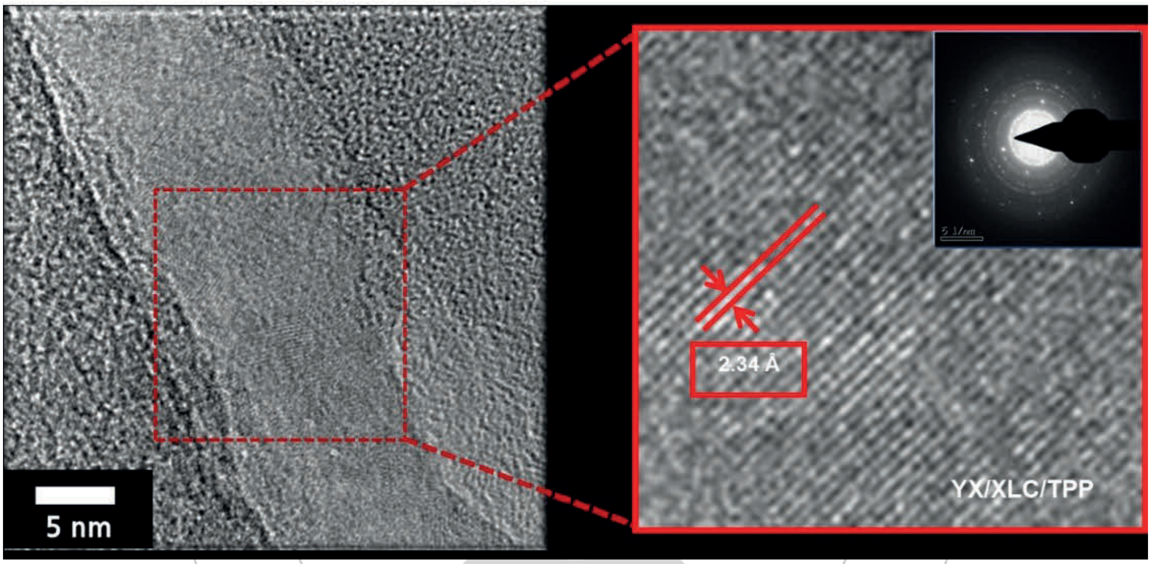
Ho Gyu Yoon

Department of Materials Science and Engineering, Korea University, Korea

Epoxy molding compound (EMC) plays an important role of protecting the semiconductor devices and mounting on a printed circuit board. It can be said that the characteristics of a semiconductor device could be partially determined by the reliability and workability of EMC. In this symposium, major reliability and workability related to EMC encapsulated semiconductor package were reviewed, and the characteristics and performance of major components composed of EMC to achieve those properties were described. A method for obtaining the curing reaction type, reaction order, and rate constants of epoxy, a crosslinked polymer, which is the basis of the workability of EMC, was presented, and the Kissinger equation was used for the calculation of relative B-stage. The WLF (Williams-Landel-Ferry) equation combined with the cure kinetics and measured gelation times at several temperatures could be applied for finding theoretical change of viscosity. Theoretical thermal conductivity (T/C) shows that an increase in T/C of the epoxy resin is more effective than high loading of filler such as alumina, which has been experimentally proven by introducing liquid crystalline epoxy. Several reliability and workability were also discussed in detail.

Figure 1. Synthesis and characterization of liquid crystalline epoxies.
Figure 2. Quasi-crystalline structure of liquid crystalline epoxy.


• Diglycidyl ether of 4,4'-biphenol epoxy (DGEBP)
OH
OH
Dihydroxybiphenyl
Epicholorhydrin
Cl
O
Reflux for 4 hours
+BTMA for catalyst at 100 °C
DGEBP
5
4
3
2
1
2
1
3
4
5
9 8 7 6 5 4 3 2 1
PPM (δ)
DGEBP
DHB
Transmission (a.u.)
4000 3500 3000 2500 2000 1500 1000
Wavelength (cm^{-1})
2800-3300 cm^{-1} O-H stretch Hydroxyl group
2900-3100 cm^{-1} 1500 cm^{-1} Aromatic ring
1240 cm^{-1} C-O-C stretch Ether group
915 cm^{-1} Epoxide group
• Bis[4-(2,3-epoxypropoxyphenyleneininomethyl)]2,2'-dimethylbiphenylene
OH
CHO
H₂N
NH₂
Reflux for 6 hours
+ Toluene sulfoic acid for catalyst
HO
OH
+Epi
+ BTMA for catalyst at 110 °C
bis[4-(2,3-epoxypropoxyphenyleneininomethyl)]2,2'-dimethylbiphenylene
(BMPE)
8
7
6
5
2
1
9
3
4
1
2
3
4
5
6
7
8
9
9 8 7 6 5 4 3 2 1
PPM (δ)
BMPH
BMPE
Transmission (a.u)
4000 3500 3000 2500 2000 1500 1000
Wavelength (cm^{-1})
2800-3300 cm^{-1} O-H stretch Hydroxyl group
1600 cm^{-1} N=CH stretch Azomethine group
1210 cm^{-1} C-O-C stretch Ether group
930 cm^{-1} Epoxide group


5 nm
2.34 Å
5 1/nm
YX/XLC/TPP

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

Special Symposium by Mid-career Biomaterials Scientists

Room 101 THU 17:40

Chair: Jin-Woo Oh (Pusan National University)

Universal Suzuki–Miyaura Catalyst-Transfer Polymerization for Precision Synthesis of Strong Donor/Acceptor-Based Conjugated Polymers

Tae-Lim Choi

Division of Chemistry, Seoul National University, Korea

Catalyst-transfer polymerization has revolutionized the field of polymer synthesis due to its living character, but for a given catalyst system, the polymer scope is rather narrow. Herein we report a highly efficient Suzuki–Miyaura catalyst-transfer polymerization (SCTP) that covers a wide range of monomers from electron-rich (donor, D) to electron-deficient (acceptor, A) (hetero)arenes by rationally designing boronate monomers and using commercially available Buchwald RuPhos and SPhos Pd G3 precatalysts. Initially, we optimized the controlled polymerization of 3,4-propylenedioxythiophene (ProDOT), benzotriazole (BTz), quinoxaline (QX), and 2,3-diphenylquinoxaline (QXPh) to modulate the reactivity and stability of the monomers. As a result, PProDOT, PBTz, PQX, and PQXPh were prepared with controlled molecular weight and narrow dispersity ($Đ < 1.29$) in excellent yield. A detailed investigation of the polymer structures using 1H NMR and MALDI-TOF spectrometry supported the chain-growth mechanism and the high initiation efficiency of the SCTP method. In addition, the use of RuPhos–Pd showing excellent catalyst-transfer ability on both D/A monomers led to unprecedented controlled D–A statistical copolymerization, thereby modulating the HOMO energy level and band gap energy of the resulting copolymers. Moreover, to demonstrate the living nature of SCTP, various combinations of D–A and A–A block copolymers (PBTz-b-PProDOT, PQX-b-PProDOT, and PQX-b-PBTz) were successfully prepared by the sequential addition method. Finally, simple but powerful one-shot D–A block copolymerization was achieved by maximizing the rate difference between a fast-propagating pinacol boronate donor and a slow-propagating acceptor to afford well-defined poly(3-hexylthiophene)-b-poly(benzotriazole).

Symposium : **POLY1-1**
Special Symposium by Mid-career Biomaterials Scientists
Room 101 THU 15:40
Chair: Won-Gun Koh (Yonsei University)

Biomaterials-based cellular reprogramming and stem cell differentiation for personalized regenerative medicine

Soo-Hong Lee

Department of Medical Biotechnology, Dongguk University, Korea

I would like to introduce recent works about cellular reprogramming and stem cell differentiation through the specific interaction of stem cells and biomaterials for personalized regenerative medicine. Understanding the biophysical relationships between stem cells and applied biomaterials can facilitate the ability to control the functions and behaviours of stem cells. However, the role of biomaterials and especially 3D microenvironment in stem cell biology remains largely unexplored, compared with that of 2D cell-culture environment. In the first topic, I would like to introduce 3D hydrogel systems to accelerate cellular reprogramming. On the other hand, in the second topic, I will introduce a novel technique for mesenchymal stem cells (MSCs) isolation from pluripotent stem cells (PSCs) by utilizing specific integrin interaction of MSC on a biomaterial. In addition, I will briefly introduce recent my works about various approaches for personalized regenerative medicine. Therefore, I believe these approaches would be useful to prepare a standard protocol providing personalized and therapeutic stem cells in regenerative medicine.

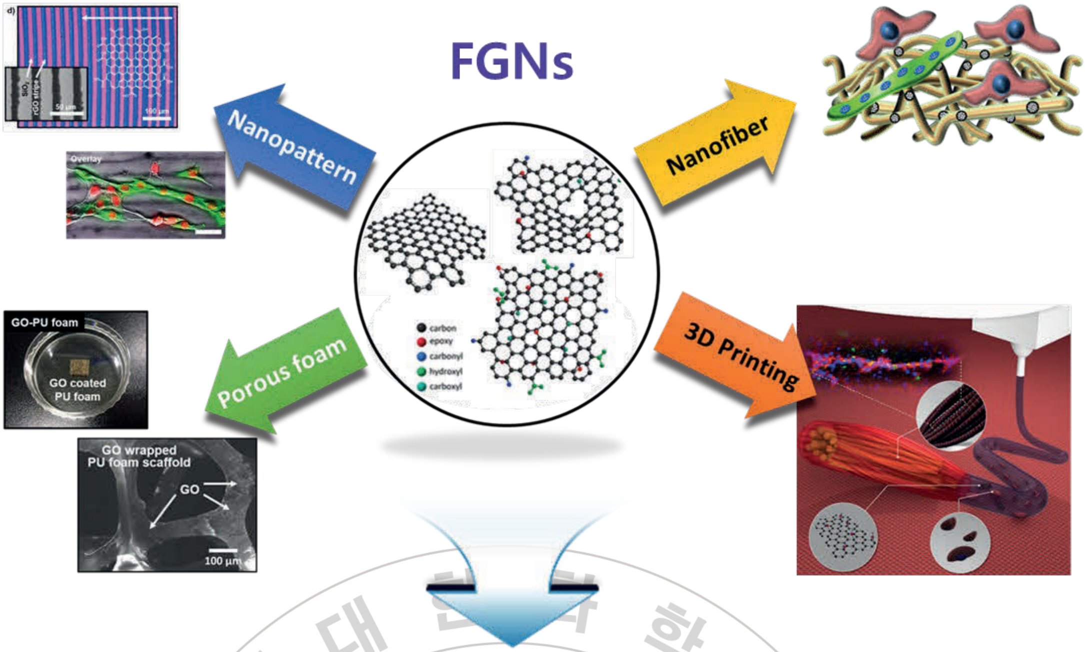
Symposium : **POLY1-2**
Special Symposium by Mid-career Biomaterials Scientists
Room 101 THU 16:10
Chair: Won-Gun Koh (Yonsei University)

Promotion of Myogenesis in Graphene-Incorporated 2D Substrates and 3D Scaffolds

Dong-Wook Han

Department of Optics and Mechatronics Engineering, Pusan National University, Korea

During the past few decades, two-dimensional (2D) nanomaterials have attracted enormous interests due to their outstanding performance in various areas ranging from electronics, photonics, biomedicine, and energy storage/harvesting. Likewise, graphene family nanomaterials have emerged since 2010 as functional 2D materials to offer a wide spectrum of technological opportunities. Owing to their exceptional physicochemical and thermomechanical characteristics as well as biological and optoelectronical properties, functional graphene nanomaterials (FGNs) are considered to be promising for many applications especially in the biomedical fields such as drug delivery, bioimaging, biosensor, theranostics, therapeutics, and tissue engineering. Tremendous studies are still underway to employ FGNs for those biomedical applications. Some seminal studies, in particular, have endeavored to determine the behavioral changes of stem or progenitor cells when faced with specific types of FGNs-based bionanomaterials. In this presentation, I'd like to discuss the potential of some graphene-incorporated 2D substrates, such as patterned arrays and nanofibrous matrices, and 3D scaffolds including porous foams and 3D printed constructs as new innovative options for regeneration of skeletal muscle tissue together with introduction of my recent studies for the development of medical devices based on FGNs.



Development of FGN-based medical devices to promote myogenesis

Symposium : **POLY1-3**
Special Symposium by Mid-career Biomaterials Scientists
Room 101 THU 16:40
Chair: Jin-Woo Oh (Pusan National University)

Biomedical applications of stimuli responsive nanoparticles

In-Kyu Park

Department of Biomedical Sciences, Chonnam National University, Korea

Hydrogen peroxide are most potent reactive oxygen species (ROS) linked with major diseases such as cancer, and inflammatory diseases. In case of cancer, H2O2 produced during hypoxic condition in the tumor supports the cancerous cells to proliferate and metastasize to other organs. Hence, the H2O2 could be the possible therapeutic target for subsidizing the inflammatory and cancerous condition. Here, we developed a manganese dioxide based albumin nanoparticle self-assembled with cationic polymers and forming stable nanoassembly for mitigating LPS induced inflammation in mice model. Our results demonstrated that nanoassembly exhibited low cytotoxicity and remarkable scavenging of H2O2 in LPS induced macrophage cells as well as in locally inflamed paw site of mice. In systemic inflammation, nanoassembly reduced the secretion of proinflammatory cytokines like TNF-α and IL-6 and therefore led to prevention of inflammatory microglial mediated neuroinflammation.

In cancer photo-immunotherapy application, hydrogel loaded manganese dioxide based albumin nanoparticle were used along with adjuvants. Here, photothermal mediated tumor reduction in 4T1 breast cancer tumor upon near-infrared (NIR) laser irradiation were significant compared to control treatment. The manganese dioxide reduced hypoxia in the tumor, that leads to prevention of epithelial to mesenchymal transition (EMT).

Overall, manganese dioxide based albumin nanoparticles showed great potential for photothermal mediated anti-cancer therapy as well as in mitigating LPS induced inflammation. Therefore, this nanoparticle could be beneficial for future clinical applications.

Symposium : **POLY1-4**
Special Symposium by Mid-career Biomaterials Scientists
Room 101 THU 17:10
Chair: Jin-Woo Oh (Pusan National University)

Biomedical application of Polypeptide & Nanosystem for cancer therapy

Yeu Chun Kim

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

Cell-penetrating peptides (CPPs) have been widely used to deliver nucleic acid molecules. Generally, CPPs consisting of short amino acid sequences have a linear structure, resulting in a weak complexation and low transfection efficacy. To overcome these drawbacks, a novel type of CPP is required to enhance the delivery efficacy while maintaining its safe use at the same time.

Herein, artificial cationic helical peptides possess an enhanced cell-penetrating property. However, their cell-penetrability is not converted by cellular environmental changes resulting in nonspecific uptake. pH-sensitive anion-donating groups were added to a helical polypeptide to simultaneously achieve tumor targeting and pro-apoptotic activity. The mitochondria-destabilizing helical polypeptide undergoing pH-dependent conformational transitions selectively targeted cancer cells consequently disrupting mitochondrial membranes and subsequently inducing apoptosis. And we report an artificial apoptosis-inducing polypeptide that destabilizes the mitochondrial membrane and transports calcium ions into the cytosol, thereby synergistically creating severe oxidative conditions. The oxidative stress highly activates an apoptotic signaling cascade, and also inhibits cell migration and invasion in vitro and in vivo. The suggested strategy for simultaneous mitochondrial disruption and perturbed calcium homeostasis demonstrates the applicability of polypeptide-based therapeutics as potent apoptosis-inducers in cancer therapy.

Symposium : **POLY2-1**
Recent Trends in Patterning Materials
Room 101 FRI 09:00
Chair: Do-Hoon Hwang (Pusan National University)

Photolithographic approaches for OLED pixel patterning

Byung Jun Jung*, Jin-kyun Lee[1,*]

Department of Materials Science and Engineering, University of Seoul, Korea
[1]*Department of Polymer Science & Engineering, Inha University, Korea*

Now, the market of organic light emitting display (OLED) is expanding from the mobile display to the large area display such as TV. The resolution of OLED has been developed through the fine metal mask with very tiny holes and extremely thin thickness. To virtual reality (VR) or augmented reality (AR) display, a higher resolution than those of current OLEDs is needed. The fabrication, quality control and maintenance of the fine metal mask become one of very difficult tasks in OLED industry. Therefore, some researchers have investigated other patterning methods.Photolithography is a conventional and well-established patterning method in silicon based electronics. In organic electronics, it is not easy to apply photolithography due to the damage or dissolution of organic layers during several steps in photolithographic process. As we know, the water and fluorinated solvents cannot dissolve the organic layers. Water soluble photoresist or fluorinated photoresist can be applied to patterning OLED layers. In this presentation, the materials and processes of photolithographic patterning in OLED will be introduced and discussed.Acknowledgements: This research was supported by the MOTIE (Ministry of Trade, Industry & Energy (project number #20012622)).

Symposium : **POLY2-2**
Recent Trends in Patterning Materials
Room 101 FRI 09:25
Chair: Do-Hoon Hwang (Pusan National University)

Photoimageable Polymeric Systems to Engineer Functional Surfaces Utilizable for Lithographic Applications

Myungwoong Kim

Department of Chemistry, Inha University, Korea

In past decades, photopatterning materials have been exploited in a range of applications including integrated circuit, displays, storage materials, and so on. They have been successful to make the structures on various dimensions in micro- and nano-scales. Beyond the conventional use for the patterning, functional materials that need to be patterned are all around in general scientific and engineering fields. The key of these pattern fabrications is preserving vital functionalities for target applications. In this talk, we demonstrate a simple, mild and clean, chemically adjustable, and photocrosslinkable copolymer systems based on o-nitrobenzyl functionalities enabling us to engineer the chemical properties of surfaces of various materials. The essential chemical principles are extended to fabricate the surfaces with quantitatively controlled chemical reactivity and more importantly, spatially controlled self-assembly of block copolymer in thin film enabling simple and versatile nanopattern fabrication.

Symposium : **POLY2-3**
Recent Trends in Patterning Materials
Room 101 FRI 09:50
Chair: Byung Jun Jung (University of Seoul)

Zirconium-based photoresists for extreme ultraviolet lithography

Ji-Hyun Jang

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

With the rapid growth of the semiconductor market, nanopatterning technologies utilizing extreme ultraviolet (EUV) is promising to attain a sub-10 nm pattern for next-generation semiconductors. Conventional polymer-based photoresists suffer from relatively low EUV photon absorption and pattern collapse. The design of new materials that can absorb a high EUV light has been suggested to enhance the properties for EUV lithography. Among the variety of materials, we have studied zirconium-based photoresist with high EUV absorption. We have synthesized a zirconium oxide-based cages as a core metal and photo-sensitive organic linkers on the surface. The zirconium-based photoresists have shown narrow particle size distribution providing the benefits for high-resolution photo-patterning. In this study, we suggest a new design of EUV photoresist for the next generation lithography technique.

Symposium : **POLY2-4**
Recent Trends in Patterning Materials
Room 101 FRI 10:15
Chair: Byung Jun Jung (University of Seoul)

Extreme UV resists based on radical chemistry of fluorinated molecules

Jin-kyun Lee

Department of Polymer Science & Engineering, Inha University, Korea

Recently, we see that lithography technology using extreme ultraviolet (EUVL) is slowly entering into the commercial production of integrated circuit (IC) chips. However, in order for EUVL to succeed in commercialization on a larger scale, it must overcome the technical challenge of 'resolution (R)-line edge roughness (LER)-sensitivity (S) trade-off dilemma'. The joint research team of Inha University and POSTECH, including the presenter, has been conducting research on the development of non-chemically amplified extreme UV resist using the radical chemistry of highly fluorinated molecules. Under high-energy EUV, a type of ionizing radiation, C-F bonds dissociate into radicals and then undergo crosslinking reactions to form an insoluble molecular network. In this presentation, I would like to report the results obtained so far for the fluorinated EUV resists that do not require reaction catalysts and additives and their potential for nano-fabrication.

Symposium : **POLY3-1**
Recent Trends in Early-career Polymer Chemists
Room 101 FRI 14:30
Chair: Myungwoong Kim (Inha University)

Polymeric Materials Inspired by Natural Polyphenols

Kyueui Lee

Department of Chemistry, Kyungpook National University, Korea

In nature, polyphenolic materials have been used for functional tools. For example, marine mussels secret sticky foot proteins having abundant phenolic molecules to fasten themselves to neighboring surfaces. Inspired by its underlying mechanisms, we were able to develop a specialized pressure-sensitive adhesive that works in extreme conditions such as underwater. Similarly, polyphenolic functional coating was developed where nucleophilic polymers can be easily grafted. For example, a thiolated polymer having anti-fouling ability can be successfully grafted on the polyphenolic coating, resulting in a novel anti-fouling surface. Applications of polyphenolic materials can be further expanded; and our lab is currently focusing on developing oxygen-responsive bioprinting materials, a supportive layer for cryo-EM, and a drug delivery platform for regenerative medicine.

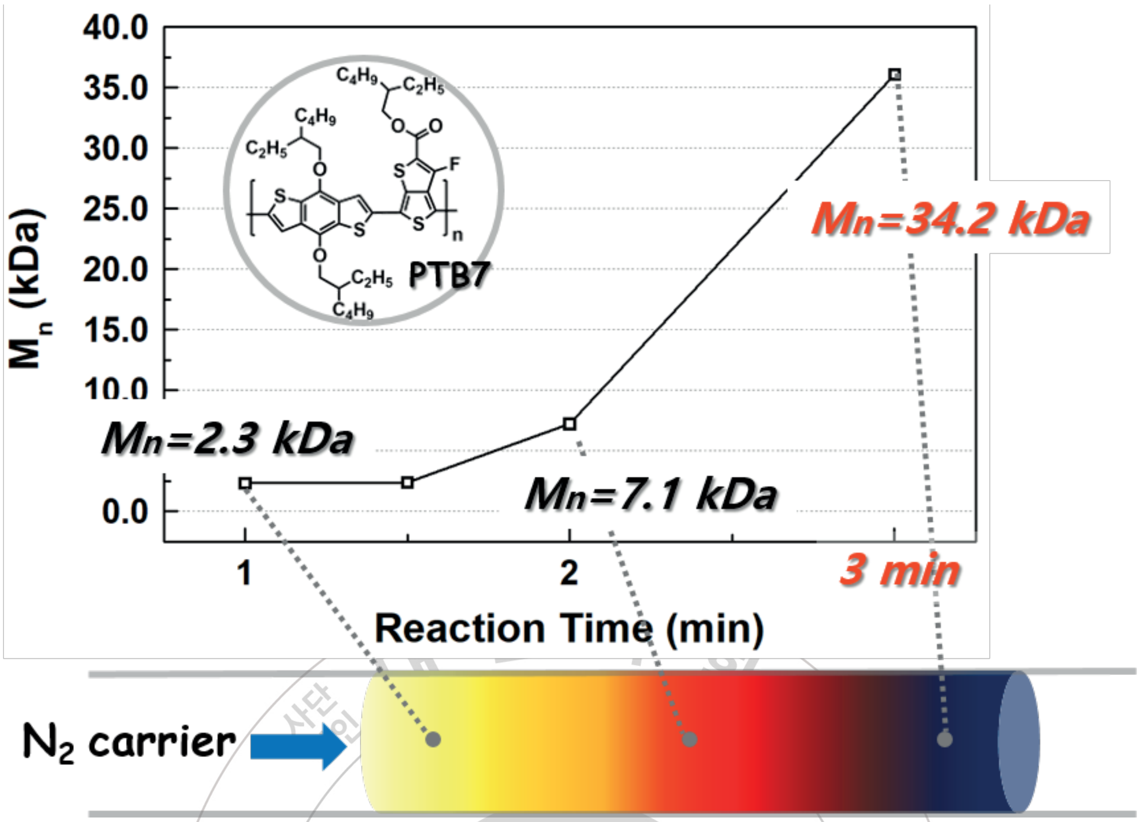
Symposium : **POLY3-2**
Recent Trends in Early-career Polymer Chemists
Room 101 FRI 14:55
Chair: Myungwoong Kim (Inha University)

Stille polycondensation in flow for the preparation of conjugated polymers

Ye-Jin Hwang

Chemical Engineering, Inha University, Korea

Much progress has been made in the development of high-performance organic electronic and photonic devices based on conjugated polymers. Molecular weight of conjugated polymer is known as a critical factor that determines material properties and device performances. However, the molecular weight of polymers synthesized from the step-growth polymerization is hard to control due to such a random polymerizing mechanism of it. To avoid this batch-to-batch variations in conventional batch reactor, we developed a flow synthesis system that can perform step-growth Stille polycondensation in a reproducible manner. By utilizing nitrogen gas as a carrier, our flow system provides uniform and precisely controlled reaction conditions without a common head and tail diffusion problem in other flow systems. We conducted Stille polycondensations to synthesize various donor (D)-acceptor (A) type conjugated polymers and monitored the polymerization process over the residence time. As an example, a representative conjugated polymer PTB7 was synthesize with a high average molecular weight (Mn) of 34.2 kDa and Đ of 1.93 in only 3 min with high reproducibility (3.1 % errors for Mn between runs).


40.0
35.0
30.0
25.0
20.0
15.0
10.0
0.0
Mn (kDa)
PTB7
Mn=2.3 kDa
Mn=7.1 kDa
Mn=34.2 kDa
1
2
3 min
Reaction Time (min)
N2 carrier

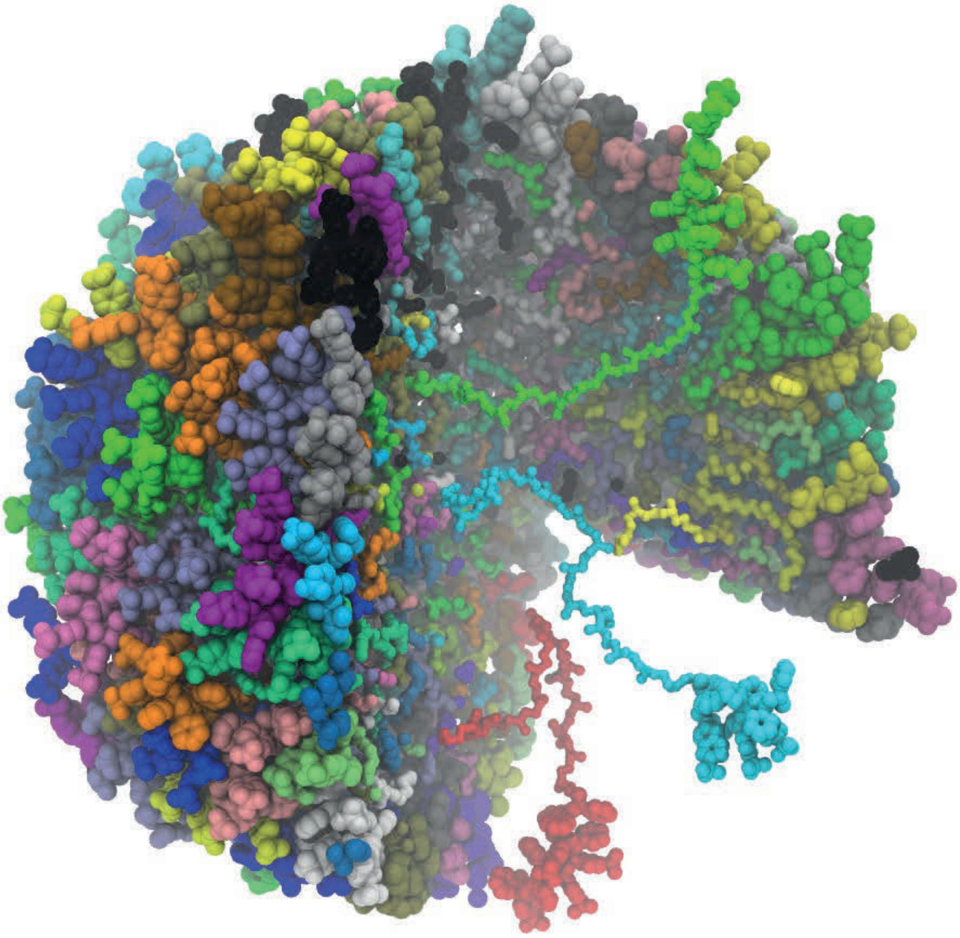
Symposium : **POLY3-3**
Recent Trends in Early-career Polymer Chemists
Room 101 FRI 15:20
Chair: Eunji Lee (GIST)

Understanding molecular driving force of self-assembly in highly charged soft materials systems via predictive molecular simulations

Chang yun Son

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

The self-assembly of surfactants and polymeric systems into ordered nanostructures is of fundamental interest in polymer physics and has practical importance to optimize the performance of the processed materials. Recently, much richer self-assembled morphologies have been reported in highly charged soft materials systems, where the strong electrostatic interaction drives unique nanostructured morphologies that are different from the conventional systems.In this work, I'll present our ongoing efforts to understand highly charged systems through predictive molecular simulations. Two unique systems will be discussed – the lyotropic self-assembly of synthetic six-tail lipidoids, and an acid-tethered block copolymer system incorporating ionic liquids. Combining molecular dynamic (MD) simulations utilizing recently developed first principles force fields along with experimental characterization, we investigate the role of the monomer structure and the ion composition in stabilizing different morphologies. Notably, the simulations show self-assembly of the synthetic lipidoids and PEs into the experimentally observed LAM, HEX and cubic structures including low symmetry A15 phase with varying conditions, illustrating the predictive power of the novel force fields. Furthermore, artificially modifying the interaction parameters and charge distribution on the molecular components reveals detailed molecular mechanism in controlling the self-assembled morphology. Our collaborative work provides novel routes to develop functional soft materials with peculiar network morphologies for biological and energy applications.



KOREAN CHEMICAL SOCIETY

Symposium : **POLY3-4**
Recent Trends in Early-career Polymer Chemists
Room 101 FRI 15:45
Chair: Eunji Lee (GIST)

Design of Narrow Bandgap Conjugated Polymers and Molecular Semiconductors for Solution-Processed Near-Infrared Photovoltaics and Photodetectors

Jaewon Lee

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

Solution-processed near-infrared (NIR) organic photodiodes have attracted recently extensive attention due to their potential applications in next-generation optoelectronics such as semi-transparent photovoltaics and NIR photodetectors. Conjugated polymers and molecular semiconductors with narrow bandgap properties are relevant as key components for the fabrication of NIR donor:acceptor bulk-heterojunction photodiodes. However, the benefits of NIR organic semiconductors remain comparatively unexplored. A critical challenge arises as one decreases optical bandgaps with respect to the counterbalance between exciton splitting and charge recombination and voltage loss in bulk-heterojunction blends. We show a rational approach to design and synthesize NIR-absorbing conjugated polymers and nonfullerene acceptors for efficient organic bulk-heterojunction devices by modulating optical bandgaps and molecular interactions.

Symposium : **INOR1-1**
Past, Present and Future of Energy Chemistry in Korea
Room 203 THU 15:40
Chair: Jin Seok Lee (Hanyang University)

Electrocatalyst for Water Oxidation and CO2 Reduction

Ki Tae Nam

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

Water splitting and electrochemical CO2 conversion are regarded as the promising approaches towards environmentally sustainable energy schemes and carbon neutrality. The oxygen evolution reaction (OER) requires extremely high overpotential due to its slow reaction kinetics. The water oxidizing cluster in photosystem II, in the form of cubical Mn4CaO5 cluster, efficiently catalyzes water oxidation. Specific questions that we intensively focus for further applications include how to translate the underlying principles in Mn4CaO5 cluster into synthetic heterogeneous catalysts. Toward this vision, we have been developing a new catalytic platform based on sub-10 nm-sized Mn oxide nanoparticles to bridge the gap between atomically defined biological catalysts. In this approach, the local atomic geometry is controlled by the surface modification of the specific ligand and the heterogeneous atom doping, that enhance the catalytic activity and selectivity. Furthermore, we detected key intermediate species, Mn(IV)=O, based on comprehensive electrokinetic and in-situ spectroscopic analysis. We revealed unique water oxidizing mechanism mediated by Mn-oxide nanocatalysts different from bulk counterparts. We further conducted electrochemical impedance spectroscopy (EIS) analysis to understand various electrochemical processes in film-type OER electrocatalysts.

The products from electrochemical CO2 reduction reaction (eCO2RR) are inevitably limited to CO, HCOOH, C2H4, and so on. Recently, we proposed new strategies for CO2 utilization, redox neutral electrosynthesis into dimethyl carbonate and nitrate coupling into amino acid. Lowering the anodic overpotential and designing the membrane-separated system are also important determinants of the overall efficiency. We explored the possibility of using counterintuitive redox-neutral reactions in eCO2RR, to expand the product scope with higher efficiency. We combined three redox cycles in undivided cell so that the input electrons do not settle in CO2, but continue to flow through the electrolyte. The mechanistic study clearly shows that the formation of methoxide intermediates and the cyclic regeneration of the homogeneous Pd-catalyst by in-situ generated oxidants are important. In addition, we developed a new electrochemical method for synthesizing a C-N bond-containing molecule avoiding usage of cyanide and amines by harnessing nitrate (NO3-) as the nitrogen source in aqueous electrolyte. To synthesize glycine, we utilized oxalic acid as carbon source which can be obtained from eCO2RR, so that our approach can provide a new route for the utilization of anthropogenic CO2 and nitrate wastes.

Symposium : **INOR1-2**
Past, Present and Future of Energy Chemistry in Korea
Room 203 THU 16:05
Chair: Jin Seok Lee (Hanyang University)

Past, Present, and Future of Korea Photovoltaic Solar Energy Society

Donghwan Kim

Materials Science and Engineering, Korea University, Korea

Solar photovoltaic technology has demonstrated a strong viability over the last 20 years or so. A significant improvement of the energy conversion efficiency from around 15% to 25% of commercial solar cells combined with the steep module price down from $4/Wp to $0.30/Wp made possible the annual installation of >100 GWp globally. Korea was an underdog in PV in terms of the technology level and the industry capacity up to 2000. The Korea's PV technology level was once estimated about 20 years behind that of the advanced countries such as Japan. Now Korea is one of the world's leading countries in the PV technologies and in the PV industry as well. As an example, Korea's PV scientists lead the world's PV R&D effort in perovskite technology by renewing the efficiency records repeatedly. The Hanwha solution ranks within the global top 5 solar manufacturer and the LG electronics produces solar cells with the highest commercial efficiencies over 24%. Korea is one of the few countries that has the whole PV value chain. Korea is also a leading country in terms of the PV installation. For example, about 4GWp of solar panel was installed in 2020 and the size ranks about 6th globally. This presentation covers the effort of Korea PV communities that made possible the brilliant achievement of today. The future direction of PV community effort will also be discussed.

Symposium : **INOR1-3**
Past, Present and Future of Energy Chemistry in Korea
Room 203 THU 16:30
Chair: Jin Seok Lee (Hanyang University)

RECENT REVIEW ON ORGANIC AND PEROVSKITE SOLAR CELLS FOR BIPV APPLICATIONS

Kwanghee Lee

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

To achieve zero-carbon or zero-energy buildings, buildings must generate energy from on-site renewable energy resources through the concept of building-integrated-photovoltaic (BIPV) systems, and also prevent energy loss to the surroundings through the use of high-performance thermal insulation materials. Moreover, such BIPV systems should be not only economic and effective but also an environmentally friendly aesthetic tool for future architecture. However, existing BIPV systems only replace the materials of conventional building envelope components such as the walls or roofs owing to the opaque and brittle characteristics of conventional photovoltaics for BIPV. Therefore, current BIPVs are unsuitable for state-of-the-art modern buildings equipped with exterior window glasses on almost all of their surfaces. To achieve zero-carbon/zero-energy consumption in future buildings, BIPVs must be consist of window-film-like PV cells with semi-transparency and flexibility for facilitating their lamination onto any exterior windows on the buildings. In this talk, I am going to address the current state of the arts of organic solar cells (OSCs) and perovskite solar cells (PSCs), which are introduced into window-film-type flexible and semi-transparent BIPV systems. Because organic semiconductors and perovskites are inherently semi-transparent in the visible region and mechanically flexible, in contrast to the opaque, brittle inorganic semiconductors used in conventional BIPVs, they are excellent candidate materials for such window-film-type BIPVs. I will also present our recent innovative method for producing high-performance flexible and transparent OPVs by integrating two types of flexible and transparent electrodes (FTEs), i.e., an ultra-thin metal and a conducting polymer as the bottom and top FTEs, respectively. Finally, the current achievements in the photostability and thermal stability issues in these promising PV systems will be reviewed and discussed.

RECENT REVIEW ON ORGANIC AND PEROVSKITE SOLAR CELLS FOR BIPV APPLICATIONS

* KWANGHEE LEE[1,2,3]
[1] *School of Materials Science & Engineering, GIST, Gwangju, Korea*
[2] *Heeger Center for Advanced Materials, GIST, Gwangju, Korea*
[3] *Research Institute of Solar & Sustainable Energy, GIST, Gwangju, Korea*

** Presenting & Corresponding Author (klee@gist.ac.kr)*

To achieve zero-carbon or zero-energy buildings, buildings must generate energy from on-site renewable energy resources through the concept of building-integrated-photovoltaic (BIPV) systems, and also prevent energy loss to the surroundings through the use of high-performance thermal insulation materials. Moreover, such BIPV systems should be not only economic and effective but also an environmentally friendly aesthetic tool for future architecture. However, existing BIPV systems only replace the materials of conventional building envelope components such as the walls or roofs owing to the opaque and brittle characteristics of conventional photovoltaics for BIPV. Therefore, current BIPVs are unsuitable for state-of-the-art modern buildings equipped with exterior window glasses on almost all of their surfaces. To achieve zero-carbon/zero-energy consumption in future buildings, BIPVs must be consist of window-film-like PV cells with semi-transparency and flexibility for facilitating their lamination onto any exterior windows on the buildings.

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Symposium : **INOR1-4**
Past, Present and Future of Energy Chemistry in Korea
Room 203 THU 16:55
Chair: Jin Seok Lee (Hanyang University)

Problems of the current research directions and desirable new research directions to mitigate the climate change

Kyung Byung Yoon

Department of Chemistry, Sogang University, Korea

Great efforts are currently being made to mitigate the ongoing climate change. For this, the conversion of various renewable energy sources to chemical energy has been considered to be an important method to help mitigate the ongoing climate change. Accordingly, various methods have been developed and tested. However, each method has its own problems. For example, during the last two decades, artificial photosynthesis has been studied extensively. However, the rate of its progress is too slow, no scalable methods have yet been developed and are not likely to be developed within a few decades in this field. Therefore, before it becomes too late, an immediate paradigm shift in the research direction has to be made. The problems of the current research directions and the desirable new research directions to mitigate the climate change will be presented.

Symposium : **INOR2-1**
Recent Trends in Inorganic Chemistry I: Organometallic Chemistry
Room 203 FRI 09:00
Chair: Min Hyung Lee (University of Ulsan)

Strategic molecular design to control photophysical characteristics of *ortho*-Carboranyl Luminophores

Kang Mun Lee

Department of Chemistry, Kangwon National University, Korea

The development for novel organic luminophores has led to considerable research into efficient functional materials for prominent optoelectronic applications. Among them, *o*-carborane (*closo*-1,2-$C_2B_{10}H_{12}$) containing organic fluorophores have been widely researched as unprecedented optoelectronic materials for a variety of photonic applications. In particular, the strong electron-withdrawing properties of the C atoms on the *o*-carborane cage lead to the formation of electronic donor–acceptor dyad systems that induce distinct intramolecular-charge-transfer (ICT) transitions with the substituted π-conjugated aromatic groups, resulting in the unique luminescent behavior. Recently, it has been extensively investigated that the ICT process involved in *o*-carboranyl derivatives can be manipulated by strategic design of molecular geometry. In line with exploring the intramolecular electronic characteristic depended on the structural feature, various *o*-carborane appended organic luminophores were prepared and their photophysical properties were analyzed in detail. Such the experimental and theoretical findings strongly suggest that the π-aromatic group appended to the *o*-carboranyl conjugate system can be used in functional optoelectronic materials showing thermally activated delayed fluorescence and visual sensory materials for detecting temperature.

Symposium : **INOR2-2**
Recent Trends in Inorganic Chemistry I: Organometallic Chemistry
Room 203 FRI 09:20
Chair: Min Hyung Lee (University of Ulsan)

Modulating the Reactivity of Metal-hydride (M-H) species for Carbon Dioxide Reduction

Ho-Jin Son

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

A critical challenge in CO2 reduction to value-added fuels and chemicals is product selectivity. Desirable CO2 products requires proton equivalents, but key catalytic Metal hydride intermediates can also be competent for direct CO2 reduction to formate/CO chemicals. Elucidating how to manage divergent reaction pathways at this central intermediate is essential to achieving high product selectivity. In our research group, diverse types of catalytic systems have been recently devised to direct the reactivity of metal hydride species for selective CO2 reduction. Herein, we describe our recent advances in realizing the efficient and selective photocatalysis in TiO2 hybrid platforms, which merge molecular component and semiconductor material to utilize merits intrinsic to each, as well as in new ligand system tuning metal's secondary coordination sphere environment.

Symposium : **INOR2-3**
Recent Trends in Inorganic Chemistry I: Organometallic Chemistry
Room 203 FRI 09:40
Chair: Min Hyung Lee (University of Ulsan)

Cobalt-Catalyzed C–O Bond Functionalization: Mechanistic Insight

Eunsung Lee

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

C–O bonds are ubiquitous in organic molecules and have been attractive alternative coupling partners of aryl halides due to various benefits such as easy accessibility and better atom economy. Therefore, there has been made a significant effort to utilize C–O bonds in aryl ethers, which involves homogeneous nickel catalysis. While investigating a cobalt catalyst for C–F bond activation in our lab,1,2 we also discovered similar cobalt catalysis for C–O bond activation, followed by borylation and silylation. Interestingly, we found that C–O bond activation involves the formation of cobalt black, which is heterogeneous catalysis. To confirm the detailed mechanistic postulation, we carried out various correlated experiments. The detailed mechanistic study will be presented.1.S. Lim, H. Cho, J. Jeong, M. Jang, H. Kim, S. H. Cho, E. Lee, Org. Lett. 2020, 7387–7392.2.S. Lim, D. Song, S. Jeon, Y. Kim, H. Kim, S. Lee, H. Cho, B. C. Lee, S. E. Kim, K. Kim, et al., Org. Lett. 2018, 20, 7249–7252.

Symposium : **INOR2-4**
Recent Trends in Inorganic Chemistry I: Organometallic Chemistry
Room 203 FRI 10:00
Chair: Min Hyung Lee (University of Ulsan)

Status of metallocene catalysts for producing high quality polyolefin and the role of SPCI

Sanghun Nam

Marketing team, SPCI, Korea

Most of the plastics including plastic molding products and plastic bags, widely used from daily life to the industrials, are made of a synthetic resin called polyolefin. The representative polyolefin are polyethylene (PE), polypropylene (PP), and elastomers.The core technology for producing polyolefin can be divided into catalysts, processes, and product designs. Among them, catalysts are regarded as key component in producing polyolefin since they can tune the properties of polyolefin as well as realizing stable plant operation and high productivity.Recently, the demand for polyolefin of high value-added products and high-quality products is growing, and for those, it is essential to synthesize metallocene catalysts having a single active site. In addition, we need different types of metallocene to produce various polyolefin for the specific purpose. In Korea, SPCI is the only company that produces metallocene catalysts, and most of the metallocene catalysts used in Korea heavily depend on overseas suppliers.SPCI is a professional company that has developed and mass-produced metallocene catalysts for 12 years, and has various synthesis methods and technologies to provide metallocene catalysts for customers safety. We will also introduce electronic materials for semiconductors, soluble-borate, and Cr catalysts for producing 1-octene based on anhydrous technology for producing metallocene catalysts.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Symposium : **INOR2-5**
Recent Trends in Inorganic Chemistry I: Organometallic Chemistry
Room 203 FRI 10:20
Chair: Min Hyung Lee (University of Ulsan)

Regioselective Cyclopolymerization of 1,6-heptadiynes Using Ru-based Olefin Metathesis Catalysts

Tae-Lim Choi

Division of Chemistry, Seoul National University, Korea

Cyclopolymerization (CP) of 1,6-heptadiyne derivatives is a powerful method for synthesizing conjugated polyenes containing five- or six-membered rings via α- or β-addition, respectively. Fifteen years of studies on CP have revealed that user-friendly Ru-based catalysts promoted only α-addition; however, we recently achieved β-selective regiocontrol to produce polyenes containing six-membered-rings, using a dithiolate-chelated Ru-based catalyst. Herein, we present our story of how we discovered that new chelated Ru catalysts could promote regioselective β-addition to produce analogous polyenes containing six-membered rings with moderate to good β-selectivity. Since then, we have focused our research on pursuing more active and β-selective regiocontrol to produce conjugated polymers with excellent β-selectivity, with a much broader range of monomers. Also, with fruitful collaboration with Mookie Baik's group at KAIST, origin of the regioselectivity was explained by DFT calculation. Lastly, we present living β-selective CP by rational engineering of the steric factor on monomer or catalyst structures. As a result, the molecular weight of the conjugated polymers from various monomers could be controlled with narrow dispersities, according to the catalyst loading. A mechanistic investigation by in situ kinetic studies using 1H NMR spectroscopy revealed that with appropriate pyridine additives, imposing a steric demand on either the monomer or the catalyst significantly improved the stability of the propagating carbene as well as the relative rates of initiation over propagation, thereby achieving living polymerization. Furthermore, we successfully prepared diblock and even triblock copolymers with a broad monomer scope.

Symposium : **INOR3-1**
Recent Trends in Inorganic Chemistry II: Bioinorganic Chemistry
Room 203 FRI 14:30
Chair: Junhyeok Seo (GIST)

Generating Circularly Polarlized Luminescence from Abiogenic Molecules

Youngmin You

Chemical Engineering and Materials Science, Ewha Womans University, Korea

Circularly polarized luminescence (CPL) refers to the differential emission between the left-handedly CPL and the right-handedly CPL. Although a human being cannot differentiate CPL from arbitrary PL, CPL is ubiquitous in nature: some animals utilize CPL for their navigation and mutual communications. Tools that generate CPL can thus aid studies of the behavioral ecology. However, conventional methods for the artificial generation of CPL are far from photonic applications as they suffer from low luminescence intensities. The challenge is to create CPL-active molecules with high luminescence quantum yields without sacrificing luminescence dissymmetry factors. As an initial approach to addressing this challenge, my group has been focusing on a supramolecular strategy. Square-planar cyclometalated Pt(II) complexes exhibit a strong propensity to form self-assemblies through pi-pi interactions. This self-assembly formation perturbs the highest-occupied dz2 orbital of the Pt center, facilitating the metal-metal-to-ligand charge-transfer (MMLCT) transition. We found that the MMLCT transition state produces strong CPL if the Pt(II) complex self-assemblies are homohelical. In order to form helical Pt(II) assemblies, we integrated the point or axial chirality into the ligand scaffolds of the Pt complexes. These synthetic approaches were found to be effective to elicit the helical sense during the self-assembly processes. The helical Pt(II) assemblies exhibit photoluminescence quantum yields and luminescence dissymmetry factors orders of magnitude greater than those of isolated Pt(II) complexes, which demonstrates the effectiveness of our approach. Finally, utility of our strategy has been further demonstrated by fabricating organic devices producing CP electroluminescence.

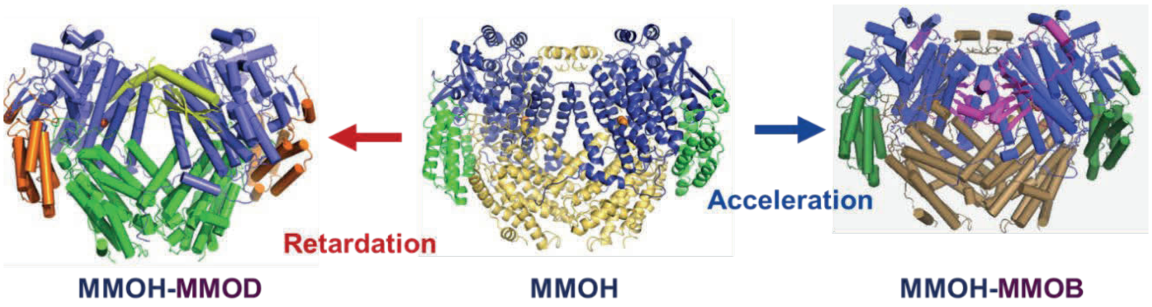
Symposium : **INOR3-2**
Recent Trends in Inorganic Chemistry II: Bioinorganic Chemistry
Room 203 FRI 14:55
Chair: Junhyeok Seo (GIST)

Allosteric Effects of Hydroxylase by Reductase and Regulatory Enzymes in Soluble Methane Monooxygenase

Seung Jae Lee

Department of Chemistry and Institute for 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.**References**1. Han Sol Jeong, Sugyeong Hong, Hee Seon Yoo, Jin Kim, Yujeong Kim, Chungwoon Yoon, Seung Jae Lee*, Sun Hee Kim*, "EPR-derived Structures of Flavin Radical and Iron-Sulfur Clusters from *Methylosinus sporium* 5 Reductase" *Inorganic Chemistry Frontiers*, **2021**, *8*, 1279–1289.2. Hanseong Kim, Sojin An, Yeo Reum Park, Hara Jang, Heeseon Yoo, Sang Ho Park, Seung Jae Lee*, Uhn-Soo Cho*, "MMOD-induced Structural Changes of Hydroxylase in Soluble Methane Monooxygenase" *Science Advances.*, **2019**, *5*, eaax0059. 3. Seung Jae Lee, Michael S. McCormick, Stephen Lippard*, Uhn-Soo Cho*, "Control of Substrate Access to the Active Site in Methane Monooxygenase" *Nature*, **2013**, *494*, 380–384.


Retardation
Acceleration
MMOH-MMOD
MMOH
MMOH-MMOB

Symposium : **INOR3-3**
Recent Trends in Inorganic Chemistry II: Bioinorganic Chemistry
Room 203 FRI 15:20
Chair: Junhyeok Seo (GIST)

Bioinorganic Strategies to Study Multiple Facets in Alzheimer's Disease

Mi Hee Lim

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

Alzheimer's disease (AD), associated with degeneration of neurons and synapses in the brain, leads to motor impairment and eventual fatality. Neurodegeneration could be related to various interconnected features, including (i) plaque formation from amyloid-β (Aβ) peptide fragments, (ii) metal ion dyshomeostasis and miscompartmentalization, as well as (iii) inflammation and increased oxidative stress due to overproduction of reactive oxygen species (ROS). The inter-relations between some of these pathological factors have been investigated. Metals are found entangled in the Aβ plaque and likely contribute to Aβ neurotoxicity and oxidative stress. ROS have been shown to increase the rate of Aβ plaque formation. Our understanding of the correlation between these elements and AD neuropathogenesis has been very limited, however. There is currently no cure for AD; therapies are focused on symptomatic relief targeting the decrease in the levels of acetylcholine, only one of the multiple factors causing the disease.[1-3] To find a cure for AD, we require a better understanding of the relationship between the various causative factors of this devastating disease. Towards this goal, we need suitable chemical tools capable of targeting and regulating its multiple underlying factors simultaneously.[2,3] Herein, our rational design and preparation of our chemical tools will be discussed with our investigations of their interactions and reactivities with targets in vitro as well as their efficacy in vivo.[4-11]References1.*Chem. Soc. Rev.* **2012**, *41*, 608.2. *Acc. Chem. Res.* **2014**, *47*, 2475.3.*Chem. Rev.* **2019**, *119*, 1221.4. *Proc. Natl. Acad. Sci. USA* **2010**, *107*, 21990.5. *Chem. Sci.* **2015**, *6*, 1879.6. *J. Am. Chem. Soc.* **2014**, *136*, 299.7. *J. Am. Chem. Soc.* **2015**, *137*, 14785.8. *Nat. Commun.* **2016**, *7*, 13115.9.*J. Am. Chem. Soc.* **2017**, *139*, 2234.10.*Proc. Natl. Acad. Sci. USA* **2020**, *117*, 5160.11.*J. Am. Chem. Soc.* **2020**, *142*, 8183.

Symposium : **INOR3-4**
Recent Trends in Inorganic Chemistry II: Bioinorganic Chemistry
Room 203 FRI 15:45
Chair: Junhyeok Seo (GIST)

Mid valent metal reactive oxygen intermediates in the oxidation reaction

Jaeheung Cho

Department of Chemistry, UNIST, Korea

High-valent metal reactive oxygen species have been widely considered as a key intermediate in various oxidative reactions of biological systems. In some examples, however, mid valent metal reactive oxygen intermediates also play important roles in biological reactions such as lipoxygenases. In this talk, we present theoretical and experimental studies of the aliphatic C-H bond activation by a mononuclear manganese(III) iodosylarene complex, [MnIII(TBDAP)(OIPh)(OH)]2+ (1). Theoretical calculations suggest that the first step of the reaction constitutes the rate-determining step, and that this step is described virtually as a hydride transfer. The hydride transfer mechanism is further supported by experimental results for the reactions of 1 with NADH analogues. Experiments also show that the hydride transfer from the NADH analogues to 1 occurs via a proton coupled electron transfer followed by a rapid electron transfer.In addition, we report the effects of redox-inactive metal ions for nitrile group activation of the peroxocobalt(III) complex with a tetradentate macrocyclic ligand, [CoIII(TBDAP)(O2)]+ (2). Unlike the previously reported nitrile activation of 2, in the presence of Zn2+, La3+, Lu3+ and Y3+, peroxyimidatocobalt(III) complexes, [CoIII(TBDAP)(R-C(=NH)O2)]2+ (R = Me (3) and Ph (4)), are generated through the reaction of 2 with nitriles. The rates of the formation of 2 are found to depend on the Lewis acidity of the redox-inactive metal ions. On the other hand, in the presence of Al3+, Sc3+ or H+ with relatively strong Lewis acidity, 2 is converted to [CoIII(TBDAP)(O2H)]2+ (5) and the reaction with nitriles did not occur. These results reveal that the reactivity and reaction pathway of the peroxocobalt(III) complex 1 in nitrile activation can be regulated by the redox-inactive metal ions and their Lewis acidity.

Symposium : **INOR3-5**
Recent Trends in Inorganic Chemistry II: Bioinorganic Chemistry
Room 203 FRI 16:10
Chair: Junhyeok Seo (GIST)

Bioinspired Nonheme Iron Complex That Triggers Mitochondrial Apop-totic Signaling Pathway Specifically for Colorectal Cancer Cells

Seungwoo Hong

Department of Chemistry, Sookmyung Women's University, Korea

A series of biomimetic first-row transition metal complexes bearing a picolylamine based water-soluble ligand were synthesized and characterized by various spectroscopic methods including X-ray crystallography and evaluated their dioxygen and ROS activation reactivity in-situ and in-vitro. It turned out that among these metal complexes, the iron complex was capable of activating dioxygen and hydrogen peroxide and pro-duced ROS species (e.g., hydroxyl radical). Upon incubation of these complexes with different cancer cells such as cervical, breast, and colorectal cancer cells such as MDA-MB-231, AU565, SK-BR-3, HeLa S3, HT-29, and HCT116 cells, only iron complex triggered the cellular apoptosis specifically for colorectal cancer cells; other metal complexes show negligible anti-proliferative activity. More importantly, those biomimetic complexes were harmless to normal cells and produced less ROS therein. The use of immunocytochemistry combined with Western blot analysis strongly supported that the apoptosis occurred via intrinsic mitochondrial pathway. The results have implications for developing novel biomimetic complexes in cancer treatments and for designing potent candidates with cancer-specific antitumor activity.

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

Advances in Materials and Surface Physical Chemistry

Room 103 THU 15:40

Chair: Sangwoon Yoon (Chung-Ang University)

Molecule-Light-Metal Interactions at Nanoscale

Zee Hwan Kim

Department of Chemistry, Seoul National University, Korea

The talk will cover the major motivation, the experimental realization, and the future direction of the research being carried out in my lab at Seoul National University. Our research goal is to experimentally study the fundamental light-molecule-metal interactions to better understand the structure-reactivity relationship of molecules on metallic surfaces at single-molecule level. For this goal, we have been studying the nano-plasmonics, the optics of resonant light-metal interaction at nanoscale, to overcome the experimental limit of molecular spectroscopy. The plasmon-enhanced spectroscopy and nanoscopy have enabled us to reveal the optical interactions between the nanoparticles and the single-molecule reaction kinetics on metal surfaces. Over the recent years, our interest has extended beyond the “classical” plasmonic interactions, leading us to explore the abnormal vibrational selection rules induced by angstrom-scale field-localization and the mechanism of unusual photocatalytic effects induced by plasmonic hot carriers.

Symposium : **PHYS1-2**

Advances in Materials and Surface Physical Chemistry

Room 103 THU 16:10

Chair: Hyun Ook Seo (Sangmyung University)

Phase Transition of Two-Dimensional Transition Metal Dichalcogenide Nanosheets to Enhance Electrocatalytic Performance

Jeunghee Park

Department of Advanced Materials Chemistry, Korea University, Korea

Phase Transition of Two-Dimensional Transition Metal Dichalcogenide Nanosheets to Enhance Electrocatalytic PerformanceJeunghee ParkDepartment of Advanced Materials Chemistry, Korea University Sejong Campus, Republic of KoreaE-mail: parkjh@korea.ac.krTwo dimensional nanosheets have recently attracted considerable attention for many applications including electrochemical catalysts and flexible optoelectronic nanodevices. Phase control of nanosheets using a heterostructure (i.e., alloy and composites) is challenging because of the band gap tunability as well as electronic structure modulation. We developed unique solution reaction method to produce the phase transition into more metallic transition metal dichalcogenide nanosheets, using the alloy phase of transition metal group V-VI-VII. The atomic arrangements were thoroughly examined using high resolution scanning transmission electron microscopy and X-ray absorption/photoelectron spectroscopy. We observed the enhanced the electrocatalytic performance of the alloy phase toward water-splitting hydrogen evolution reaction (HER). Extensive spin-polarized density functional theory calculations consistently predicted the phase transition, in agreement with the experimental results. The Gibbs free energy along the pathway of HER indicates that this enhance HER performance is mainly due to the more favorably formed vacancy sites in the alloy phase. Understanding the catalytic reaction of the phase-transition alloy phase at the atomic level would provide deep insight into the design of phase control systems.

Symposium : **PHYS1-3**
Advances in Materials and Surface Physical Chemistry
Room 103 THU 16:30
Chair: Hyun Ook Seo (Sangmyung University)

Time-resolved operando spectroscopy for photocatalysis to electrocatalysis

Wooyul Kim

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

Direct observation of key intermediates on the catalyst surface is one of the biggest challenges in various photo/electro-catalysis including CO2 reduction reaction O2 reduction reaction, etc. For a rational understanding of the reaction mechanism, combined studies encompassing complementary tools such as electrochemical characterization, computational calculations and operando spectroscopies should be conducted. Among various operando spectroscopies, the time-resolved attenuated total reflection-surface enhanced infrared absorption spectroscopy (ATR-SEIRAS) is particularly suitable for the investigation of electrochemical CO2RR as it allows observation of interfacial processes in real-time owing to its high surface sensitivity. Additionally, time-resolved analysis would reveal the kinetic relevancy of intermediates and their relationship with the reactants and the products based on their dynamic behavior during the reaction. Lastly, a combination of the operando spectroscopic studies with material characterization would enable a correlation of the behavior of the intermediates and the catalyst conditions. Herein, I will introduce in situ time-resolved FT-IR (or ATR mode) spectroscopic techniques to acquire the isotopically labeled products and key intermediates from the photoreduction of carbon dioxide.

Symposium : **PHYS1-4**
Advances in Materials and Surface Physical Chemistry
Room 103 THU 17:00
Chair: Han-Kyu Choi (Kunsan National University)

Surface Chemical Modification of 2D Materials for Tuning Electronic and Optical Properties

Hyunseob Lim

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

Research interest into two dimensional (2D) materials other than graphene has recently become intense, first because of the basic desire of researchers to explore new worlds in two dimensions from the point of view of materials research, and second to avoid the drawbacks of graphene for certain applications. Compared to metallic property of graphene, hexagonal boron nitride (h-BN) and transition metal dichalcogenides (TMDs) have insulating and semiconducting properties, respectively. Therefore, these 2D materials can be widely used for various applications regarding to their unique properties. Here, I present the recent research results working on graphene, and 2D transition metal dichalcogenides. The presentation includes the novel approaches for surface chemical modification on 2D materials for modulating their electrical and optical applications. 1) Novel chemical route was developed to synthesize centimeter-scale stoichiometric “graphenol (C6OH1)”, a 2D crystalline alcohol, via vapor phase hydroxylation of epitaxial graphene on Cu(111). Atomic resolution scanning tunneling microscopy revealed this highly-ordered configuration of graphenol and low energy electron diffraction studies on a large-area single crystal graphene film demonstrated the feasibility of the same superstructure being achieved at the centimeter length scale. 2) An electrochemical approach was also developed for facilitating direct surface functionalization of 2H-MoS2 with 4-bromobenzene diazonium tetraborate (4-BBDT). Successful functionalization was characterized using various microscopic and spectroscopic analyses

Symposium : **PHYS1-5**

Advances in Materials and Surface Physical Chemistry

Room 103 THU 17:20

Chair: Han-Kyu Choi (Kunsan National University)

Plasmonic-induced fluorescence resonance energy transfer for spectrum conversion

Doo-Hyun Ko

Department of Chemistry, Sungkyunkwan University, Korea

The conversion and manipulation of light via lanthanide-based upconversion (UC) and downshifting (DS) show promise in numerous applications. We demonstrate the lanthanide-doped nanotemplates to improve conversion of ultraviolet and near-infrared to visible light through resonant-mode excitation. The templates are fabricated using nanoimprint technique wherein ordered arrays of nanoscale features are readily made over large areas. The facile process and mild fabrication condition for the proposed structure has potential advantage of applying for flexible devices. It is found that optimized silver nanodisk and the conversion layer thickness match MIM (metal-insulator-metal) resonance mode and thereby result in both enhanced upconversion and downshifting luminescence. All lanthanide luminescence layers for upconversion and downshifting process enable to utilize the cavity mode for the enhanced both luminescence performance by matching emission range from both upconversion and downshifting. The structure is showing a promising way to harness the entire solar photons by converting both ultraviolet and near-infrared to visible light concurrently through resonant-mode excitation.

Symposium : **PHYS2-1**

Recent Advances in Physical Chemistry

Room 103 FRI 09:00

Chair: Ilsun Yoon (Chungnam National University)

Enhanced Photoelectrochemical Water Splitting Efficiency of BiVO4 Based-Photoelectrode by Building Phase-Junction Configuration

Woon Yong Sohn

Department of Chemistry, Chungbuk National University, Korea

Bismuth vanadate (BiVO4), one of the mineral forms of metal oxide, has been regarded as one of the best materials for a photoanode in a photoelectrochemical (PEC) cell due to its high earth abundance, non-toxicity, and the suitable value of the band gap for the absorption of visible light. However, the pure BiVO4 involves some drawbacks, which limit its use in the practical implementation, e. g. low conductivity. In order to make up for the weak aspects of BiVO4, building the heterojunction configuration has been regarded as one of the best methods to enhance the water splitting efficiency. However, because of the lattice mismatch between two difference species in the junction, the defect states could be generated, in which the charge recombination takes place. To solve this weak point of the heterojunction and enhance the photoelectrochemical performance of the BiVO4 photoanode, we designed the phase junction configuration including three types of the BiVO4 crystal structure. (Monoclinic Scheelite (MS), Tetragonal Scheelite (TS), Tetragonal Zircon (TZ))We could prepare the film including three phases, MS, TS and TZ. The PEC performances of the as-prepared samples were evaluated by observing the current densities as a function of the applied bias voltage. We demonstrated that the film (MS&TS&TZ) shows both the high current density (1.2 mA/cm2 at 1.23 V vs RHE) and the low turn on voltage (0.44 V vs RHE), compared to those of bare BiVO4 (0.68 mA/cm2 at 1.23 V vs RHE, 0.6 V vs RHE). The origin of the improvement was revealed by using one of the time-resolved spectroscopic techniques, heterodyne transient grating method (HD-TG), and photo-electrochemical impedance spectroscopy (PEIS), which will be discussed in the presentation.

Symposium : **PHYS2-2**
Recent Advances in Physical Chemistry
Room 103 FRI 09:20
Chair: Ilsun Yoon (Chungnam National University)

The role of polymer crystalline domain for exciton-dissociation

Jaehong Park

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Microstructures of conjugated-polymers in condensed-phase have shown to play important roles on governing the performance of polymer-based optoelectronics. We prepared highly-ordered crystalline poly(3-hexylthiophene) particle (P3HT-CP), made with regioregular P3HT (regioregularity＞99%) by slow antisolvent diffusion method. Various particle characterization data, including SEM and TEM and x-ray diffraction analysis verified the high degree of crystalline formation, revealing continuous crystalline domains extending over 100s nm scale. Electronic absorption spectroscopy and excited-state dynamics based on fluorescence and ultrafast transient absorption spectroscopy for the P3HT-CP will be discussed. These microscopic and optical spectroscopic results suggest enhanced crystallinity in P3HT-CP, which could be a model system to understand exciton dynamics in polymer crystalline domains and the role of polymer microstructures.

Symposium : **PHYS2-3**
Recent Advances in Physical Chemistry
Room 103 FRI 09:40
Chair: Ilsun Yoon (Chungnam National University)

Frontiers in Sequencing and Imaging-based Methodologies for Single-cell Analysis

Chang Ho Sohn

Advanced Science Institute, Yonsei University, Korea

All cells are different. Starting from the same genetic information, every cell functions differently but harmoniously, together in place via cell-cell interactions. In diseases, such functions are disrupted and cells behave abnormally with high heterogeneity. To understand diseases such as cancers that possess highly diverse genetic features, it is important to investigate their heterogeneity at the single-cell level. Recent advances in single-cell analyses by next-generation sequencing and tissue clearing technologies have broadened our understanding about how complex biological systems work. Yet, current single-cell methods are unable to detect isoforms or post-translation modifications of proteins, which play significant roles in cell signaling pathways whose malfunctions often lead to the onset of many diseases. Also, to fully understand the biological status of the samples, investigating both mRNA and proteins in situ is critical. However, consolidated tissue clearing/expansion methodologies for the simultaneous preservation of various tissue features including tissue architectures, fluorescent proteins, antigenicity of proteins, and nucleic acids have not been reported. I will present my recent works in the development of novel single-cell analysis platforms to address the challenges described above and discuss the future directions toward their applications for spatial multi-omics in various biological systems.

Symposium : **PHYS2-4**
Recent Advances in Physical Chemistry
Room 103 FRI 10:00
Chair: Ilsun Yoon (Chungnam National University)

Light management with surface microwires structure for c-Si photovoltaics

Kwanyong Seo

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

Silicon microwires are very promising candidates for next-generation photovoltaics. Si microwires achieve strong broadband light absorption, acting as an antireflection coating layer. In addition to superior optical properties, Si microwires can effectively separate and collect photocarriers at the radial junction owing to a short diffusion length. This factor can relax the requirement for high-quality materials, enabling a reduction in the cost of producing solar cells. In this talk, I will review recent progress in vertically aligned Si microwire photovoltaics with reference to (1) optimized microwire structures to enhance light absorption, (2) uniform radial junctions for effective carrier separation, (3) minimization of surface recombination through surface treatments, and (4) fine metal electrodes for efficient carrier collection. In addition, we present studies on flexible crystalline Si photovoltacis that use mechanically flexible Si microwires.

Symposium : **PHYS2-5**

Recent Advances in Physical Chemistry

Room 103 FRI 10:20

Chair: Ilsun Yoon (Chungnam National University)

Perovskite-type Oxynitrides $AB(O,N)_3$ for Solar Water Splitting

Jeongsuk Seo

Department of Chemistry, Chonnam National University, Korea

Photocatalytic (PC) and photoelectrochemical (PEC) water splitting using semiconductors have been a potential means of directly producing renewable hydrogen from water. The semiconductors capable of absorbing a wide wavelength range of visible light are necessary to enhance the solar-to-hydrogen (STH) conversion efficiency. The n-type perovskite oxynitrides, $AB(O,N)_3$ (A=La, Ca, Sr, or Ba and B=Ti, Ta, or Nb) are photo-responsive to wavelengths longer than 600 nm (band-gap energies E_g; 1.7~2.1 eV), leading to theoretically STH conversion efficiency above 10%. Band edge potentials of the oxynitrides straddle water redox potentials so that these materials drive solar-driven overall water splitting thermodynamically. E_g of the $AB(O,N)_3$ can also be tuned by employing different combinations of A- and B-site cations. However, the water splitting over the perovskite oxynitrides remains still low. Herein we present effective synthesis of less-defective $AB(O,N)_3$ for high PC and PEC water splitting activity under visible light irradiation. Surface and bulk characterizations of the perovskite $AB(O,N)_3$ prepared by different synthetic approaches and the corresponding water splitting activity will be discussed in the presentation.

Symposium : **PHYS2-6**
Recent Advances in Physical Chemistry
Room 103 FRI 10:40
Chair: Ilsun Yoon (Chungnam National University)

Electrochemical CO2 reduction over Au-modified metal oxide electrodes in experimental physical chemistry approaches

Youngku Sohn

Department of Chemistry, Chungnam National University, Korea

Conversion of CO2 into recycled energy fuels by electrochemistry has been a very attractive potential strategy for solving both energy and environmental issues. This talk introduces electrochemical CO2 reduction method over diverse electrode materials and more focuses on electrochemical CO2 reduction products over Au-modified metal oxide electrodes showing new CO2 reduction products. The reaction channels are deeply discussed with experimental physical chemistry concepts by aid of X-ray photoelectron spectroscopy, ultraviolet photoelectron spectroscopy, X-ray diffraction crystallography, scanning electron microscopy, transmission electron microscopy, and Raman spectroscopy.

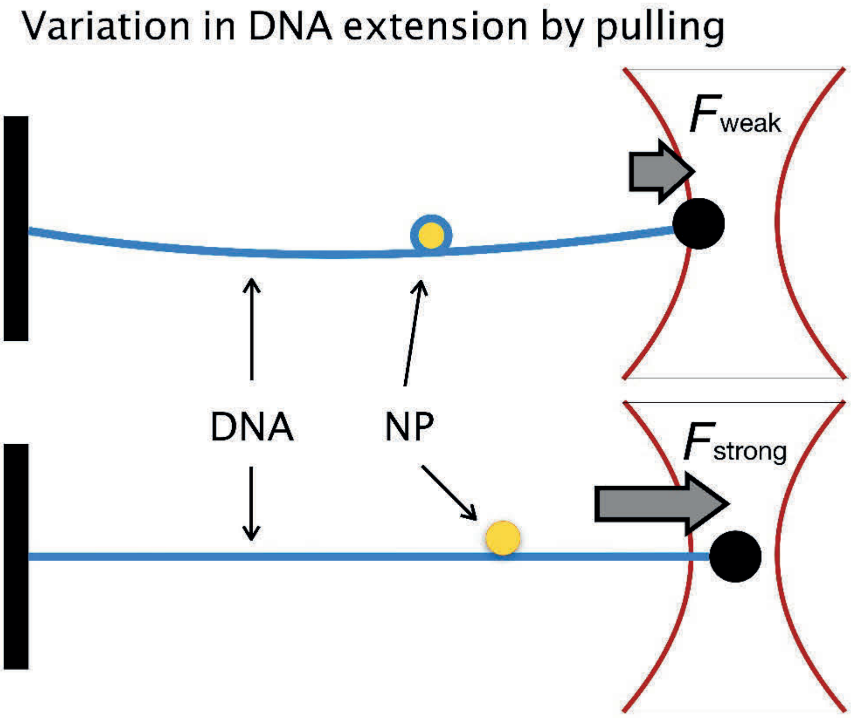
Award Lecture in Division : **PHYS3-1**
Advances in Theoretical and Computational Chemistry
Room 103 FRI 14:30
Chair: Sangwoon Yoon (Chung-Ang University)

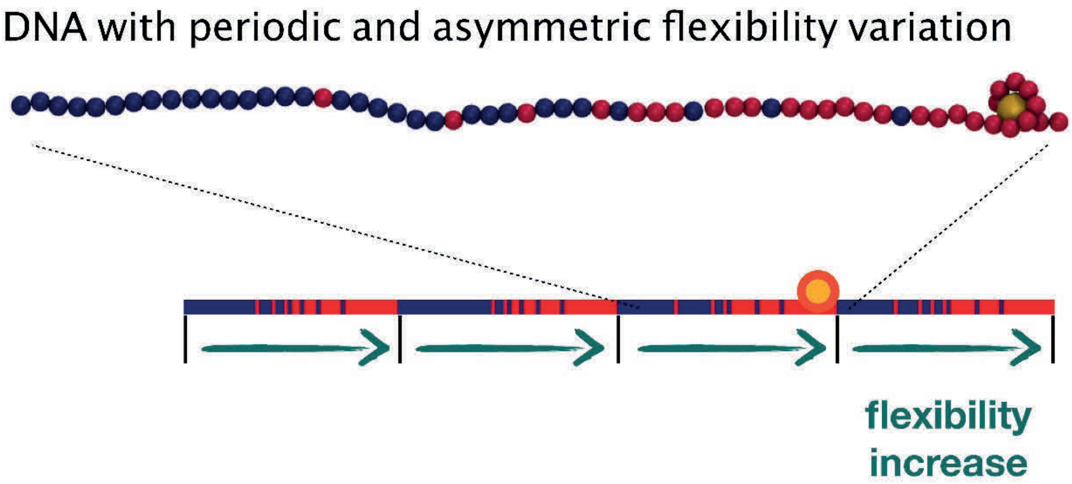
Computational design for DNA-based nanoscale Brownian motors driven by nonequilibrium fluctuations

Jun Soo Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

In this presentation, we introduce our efforts to develop DNA-based nanoscale motors using computer simulations of DNA models at various scales. For the purpose of DNA-based nanoscale motors, sequence-dependent flexibility variation of double-stranded DNA is a critical tool for the development of an asymmetric potential that is required to bias the random Brownian motion. First, we discuss a recently proposed DNA-based Brownian motor for directional nanoparticle delivery. We showed that a cationic nanoparticle moves in a specific direction along double-stranded DNA with gradual flexibility variation. By generating nonequilibrium fluctuations in terms of repetitive exchange of solutions with different salt concentrations or repetitive DNA stretching and relaxation, we propose that cationic nanoparticles bound to double-stranded DNA with periodic and asymmetric flexibility variation can be delivered in a specific direction along a single, long DNA molecule. Secondly, we discuss our recent studies on a circular, double-stranded DNA molecule with short lengths, called the DNA minicircle. DNA minicircles with ≤100 base pairs have a variety of potential applications in the development of DNA-based molecular machines, composed of DNA catenanes and rotaxanes. We showed that the sequence-dependent flexibility influences DNA structural properties including twisting and defect formation. These works propose novel utilities of DNA molecules in nanoscale applications based on sequence-dependent DNA mechanics.


Variation in DNA extension by pulling
F_{weak}
DNA
NP
F_{strong}


DNA with periodic and asymmetric flexibility variation
flexibility increase

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

Advances in Theoretical and Computational Chemistry

Room 103 FRI 14:55

Chair: Sangwoon Yoon (Chung-Ang University)

Structure and phase transitions of the electric double layer

Hyungjun Kim

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

Electrochemistry, the fundamental basis of sustainable energy conversion technologies, studies the interconversion of electric-chemical energy at heterogeneous interfaces. The electrochemical reaction mainly occurs at the solid-liquid (or electrode-electrolyte) interface, where a characteristic liquid structure, i.e., an electric double layer (EDL) is formed. Since the early 1900s, when the concept of EDL was first proposed, unremitting efforts have been made to identify EDL structural changes depending on the applied potential, but only a few molecular details have been disclosed to date. One famous example is EDL capacitance, an indicative quantity of the EDL structural change, which shows two characteristic peaks in a dilute electrolyte, but no molecular theory of liquid structure has fully explained them. To address this century-long debate, we develop a molecular simulation method to model the electrified interfaces based on quantum mechanical electronic structure theory and energetics – a density functional theory in classical explicit solvents (DFT-CES). Using DFT-CES, we find unprecedented liquid structural changes and phase transitions of the EDL, which originate two capacitance peaks at the same potentials to the experiment. Furthermore, we envisage a new perspective for developing better electrochemical systems by tailoring the interface; there’s plenty of room in between.

Symposium : **PHYS3-3**
Advances in Theoretical and Computational Chemistry
Room 103 FRI 15:20
Chair: Jae Woo Park (Chungbuk National University)

Characteristics of various polymers from atomistic molecular dynamics simulation

Sanghun Lee

Department of Chemistry, Gachon University Global Campus, Korea

This presentation introduces two case studies of real polymers from atomistic molecular dynamics simulation. The first is the study of polymeric thin films with various chemical structures. The calculated surface tensions of polyethylene, polytetrafluoroethylene, polystyrene, and poly(alkyl methacrylate)s from statistical mechanical virial tensor equation are in good agreement with experimental results, which provides good support for the force field parameters employed. Through the analysis of density profiles of specific atoms and orientational order of backbones or substitutes, detailed atomistic structures of thin films are well understood in the sub-nanometer length scale. The second study is a plastic deformation of semicrystalline polyethylene. It is confirmed that the plastic deformation behavior is strongly influenced by the rate of strain whereas the elastic modulus is almost independent of the rate. The classical theory of plastic deformation is revisited in terms of stress-strain curve, crystallinity, and entanglements.

Symposium : **PHYS3-4**
Advances in Theoretical and Computational Chemistry
Room 103 FRI 15:40
Chair: Jae Woo Park (Chungbuk National University)

Materials Data eXplorer: web-based data service for advanced data-driven research in chemistry community

Jungho Shin, Hyunju Chang[1,*]

Chemical Data-driven Research Center, Korea Research Institute of Chemical Technology, Korea
[1]*chemical data driven research center, Korea Research Institute of Chemical Technology, Korea*

Data-driven approach as the fourth paradigm in science helps chemists to understand materials properties that can be described by the relationship among materials data and discover new materials in the field of chemistry. As many similar and different databases which are designed for this purpose have been developed for the last 20 years and they all are dispersed over the world, integration and classification of materials information from multiple databases is needed for the advanced data-driven approach.Materials Data eXplorer, MatDX, has been developed as a user-friendly web-based interface, in the concept of a data warehouse solution which can be a useful strategy for connecting multiple databases. Using material tags can be found on this web service, researchers can quickly and easily search for interesting materials and view detailed information about composition, structure, properties and applications. Analysis functionality visualizes statistical relationships between materials data in an interactive way.The most important aim of these services is clearly to enable researchers to discover new candidates for targeted properties based on data of numerous materials in the chemistry community. MatDX including two sub-categories of PubDX (for the published data) and CalcDX (for the calculated data), is now ready to be used through http://materials.chemdx.org.

Symposium : **PHYS3-5**
Advances in Theoretical and Computational Chemistry
Room 103 FRI 16:00
Chair: Jae Woo Park (Chungbuk National University)

MRSF and REKS for Strong Electron Correlations

Cheol Ho Choi

Department of Chemistry, Kyungpook National University, Korea

The major assumption behind the standard Kohn-Sham (KS) methodology is that the exact ground state of any fermionic system can be exactly mapped on the ground state of a system of non-interacting (quasi-)particles moving in an external potential modified in such a way that the density remains invariant. This assumption however has been challenged, since not any physical fermionic density can be mapped on a non-interacting pure-state due to strong electron correlations.It has been found that the challenges can be overcome through either at the level of response theory – the MRSF method, or at the level of self-consistent field theory – the REKS method (a variant of ensemble DFT) not only for ground but also excited electronic states. As a result, MRSF and REKS can be a method of choice not only for simple closed shell systems, but also for challenging multi-reference open shell situations such as singlet diradicals, bond dissociations, conical intersections, etc.

Symposium : **PHYS3-6**

Advances in Theoretical and Computational Chemistry

Room 103 FRI 16:20

Chair: Jae Woo Park (Chungbuk National University)

Recent Advances in Density-Corrected Density Functional Theory

Eunji Sim

Department of Chemistry, Yonsei University, Korea

The significance of density-corrected DFT (DC-DFT) is that it can help systematic development of approximate density functionals by providing the principle of determining true error. The exact universal functional has zero error in the functional form, so it also has no density error. The framework of DC-DFT points out that there exist two errors in all self-consistent DFT calculations caused by approximate functional and approximate density. Conventional DFT error analysis is based on total energy errors and cannot identify the cause of the error or determine the accuracy of the functional. DC-DFT uses more accurate densities instead of self-consistent densities to reduce density-driven errors and, at the same time, properly evaluate functional errors. In this talk, the framework of DC-DFT is reviewed and presented with applications ranging from strong interactions such as covalent bonds to weak interactions such as torsional barrier energy, including hypothesis testing of DC-DFT.

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

Recent Studies in Bioanalyses Using Non-human Subjects

Room 104 THU 16:50

Chair: Tae-Young Kim (GIST)

Mass Spectrometry and Metrology in Chemistry

Hun-Young So

Shimadzu Scientific Korea, Korea

Mass spectrometry has been developed as a powerful analytical tool routinely used in laboratories carrying out wide variety of routine chemical analysis. It is also one of essential instruments used for certification of reference material in high purity form or in matrices. Isotope dilution mass spectrometry is often used as an absolute tool for certification of reference materials. Mass spectrometry is also used to monitor isotopic composition of certain element contained in raw materials used to be prepared as a candidate of reference materials. In any chemical measurement (analysis), evaluation of uncertainty of measurement result is only possible by using reliable reference materials and is regarded as an inevitable job of a laboratory for demonstration of its competence and reliability in analytical service provided for customers. This talk will include the relationship of metrology to mass spectrometry with personal experiences acquired by contributing the foundation of a global community of metrology in chemistry with his knowledge on mass spectrometry as major research area.

Award Lecture in Division : **ANAL1-6**
Recent Studies in Bioanalyses Using Non-human Subjects
Room 104 THU 17:05
Chair: Tae-Young Kim (GIST)

Analytical Science as a core technology of industry

Hye Sung Cho

LG Energy Solution, Korea

Chemical Analysis is very important for the development of new products, processes or quality control and to solve material-related problems in a chemical company. As the information, it provides, affects major decisions or R&D direction in many ways, analytical laboratory is the core functional research unit in a chemical R&D. With over 32 years of research experience in the materials characterization division of industrial R&D, the complicated role of analytical laboratory in chemical industry is going to be presented.

Award Lecture in Division : **ANAL1-7**
Recent Studies in Bioanalyses Using Non-human Subjects
Room 104 THU 17:20
Chair: Tae-Young Kim (GIST)

Biomarker Discovery and Diagnostics for Human Health

Wonryeon Cho

Department of Chemistry, Wonkwang University, Korea

Cancer, one of the refractory diseases, is still a challenging problem for all of mankind. Targeted glycoproteomics using affinity chromatography (AC) was used to identify and quantify cancer-related glycoproteins with cancer and normal plasma from breast cancer and colon cancer patients in U.S.A. Then after returning to Korea, AC was used to isolate and identify potential cancer biomarker glycoproteins by targeting disease-associated glycans between cancer patients and healthy control groups. For this research, several types of cancer patients' plasma were collected from several hospitals and lung cancer was at first studied on the basis of traditional Korean medicine. Then colon cancer biomarkers were found using self-packed Con A and SNA serial affinity chromatography in human plasma. Exosome proteins in plasma were also discovered in lung cancer patients. Recently, prostate cancer tissues have been used for better biomarkers using PSA As a control group for cancer patients, healthy elderly people were evaluated and categorized based on aging and exercise levels in elderly yoga programs through lectin based glycoproteomics, which was consistent with the triglyceride and glucose (TyG) Index used in the doctor's office. The potential of these candidates as cancer biomarkers remains to be validated in much larger and more diverse populations of cancer patients. Sample Displacement Chromatography (SDC) was also developed for glycan heterogeneity differentiation in cancer biomarker discovery. Efficacy of natural antibacterial feeds were also evaluated for aquaculture using proteomics.

The ultimate goal is to develop simple and economical cancer diagnostics kits by immobilizing cancer-related proteins in plasma on the biocompatible coatings for human health. The disease diagnostic kits have several selected antibodies which can be immobilized on the inorganic surfaces with their native structures for their activities. As a result, biocompatible polymer coatings were used to build up nanostructures on these surfaces and then applied to BioCD products and chromatography columns for commercial use.

Symposium : **ANAL1-1**
Recent Studies in Bioanalyses Using Non-human Subjects
Room 104 THU 15:30
Chair: Wonryeon Cho (Wonkwang University)

Multi-omics approaches to investigate responses of olive flounder with infectious disease.

Suhkmann Kim

Department of Chemistry, Pusan National University, Korea

Streptococcus parauberis (S. parauberis) and viral hemorrhagic septicemia virus (VHSV) are the most common infectious diseases affecting olive flounder (Paralichthys olivaceus) in South Korea. This study comprehensively investigated the responses that occur in the host body of infected fish by omics analysis including transcriptomics, proteomics, and metabolomics. We conducted experimental infections for bacteria and viruses and the infection rate and cumulative mortality were confirmed. Sampling was performed on 3- and 7-days post-challenge (DPC) for S. parauberis infection and 3,7, and 14 DPC for VHSV infection. Omics analysis were performed targeting the head kidney, which has a major immune function. The transcriptomic changes in the head kidney based on RNA-seq. The proteins were analyzed with nano-scale liquid chromatographic tandem mass spectrometry (nLC-MS/MS) and protein database searches. In addition, metabolomics enables the determination of the levels of small metabolites in intact tissues using high-resolution magic angle spinning (HR-MAS) NMR. Omics analysis in S.parauberis-infected fish revealed activated stress response and decreases in the expression of genes and metabolites in immune system at DPC 3. Whereas, in DPC 7, energy metabolism such as glycolysis and TCA cycle, and response to bacteria was increased, which this may be correspondence mechanism of host of bacterial infection. For VHSV infection, the expression of genes and metabolic pathway related to innate immune system was increased at DPC 3. During the lately stage of infection, the antioxidant response and energy metabolism were elevated at DPC 7 and 14, while MHC class I and II expression for antigen processing were downregulated, indicating the failure to resist the VHSV. Therefore, we identified the different metabolic changes depending on the type of pathogen. Based on these results, the effect of immune-enhancing biomaterials on the defense against S. parauberis was confirmed in a further study. The aim of this study was to indicate that -omics profiling can be used to manage infectious diseases in aquaculture industry; this profiling can also offer basic data for multiple uses.

Symposium : **ANAL1-2**
Recent Studies in Bioanalyses Using Non-human Subjects
Room 104 THU 15:50
Chair: Wonryeon Cho (Wonkwang University)

Quantitative proteomics reveals the mechanisms of physiological responses of marine ectotherms to environmental stressors

Tae-Young Kim*, **Woo Young Song**[1]

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

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

Survival and growth of marine invertebrates inhabiting the tidal zone are highly affected by environmental stressors. In recent years, there have been frequent incidences of mass mortality of the aquacultured ectotherms in summer, prompting speculation about physiological responses of the ectotherms against global warming and acute temperature variations. To reveal the mechanism of acclimation in two marine ectotherms-abalone and oyster, isobaric tag-based quantitative proteomics was performed. These organisms were exposed to environmental stressors with either temporal or spatial variations and analyzed by bottom-up proteomics using liquid chromatography-mass spectrometry. To overcome the lack of functional annotation for marine invertebrate proteome, the Basic Local Alignment Search Tool (BLAST) was performed between the identified protein sequence and non-redundant reference protein database. The significantly changed proteins under environmental stress were related to energy metabolism and thermotolerance. Metabolic pathway enrichment analysis provided a plausible explanation for the correlation between differential protein expression and observed physiological responses. In summary, differential protein expression of marine ectotherms provided a clue for the stress response mechanism to meet the increased energy demand and repair the cell damage.

Symposium : **ANAL1-3**
Recent Studies in Bioanalyses Using Non-human Subjects
Room 104 THU 16:10
Chair: Wonryeon Cho (Wonkwang University)

Concept and practice of chemical analysis tools in studies with drugs in aquatic animals

Kwan Ha Park

Kunsan National University, Korea

The use of chemical analysis is increasing becoming an essential component in studies with aquatic animals. For among several areas, highly sensitive and state-of the-art analytical tools may mostly be required for detection of trace amounts of toxic chemicals in animal tissues. Due to the trend of demanding more healthy and high protein foods, such works are frequently performed in order to guarantee the public safety of aquatic animal food consumers. Currently, most these analytical purposes are fulfilled usually adopting high-performance liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS). In response to meet the increasing demand of aquatic foods, we are artificially growing various aquatic animals to substitute the decrease in wild capture quota. Artificial growth in turn asks for use of some drugs to cope with the disease occurrence under unnatural environments for those animals. Although limited to certain therapeutic categories like antibiotics quite often, a number of drugs are actually in use these days. We must be able to tell that a given animal food is safe (edible) or not when on market. This acceptable safe level called maximum residue limit (MRL) is obtained from toxicological data performed in mammalian animals and/or human experience. We should not allow the harvest of hazardous cultured aquatic animals until they excrete ingested drugs below the MRL threshold. As we cannot test every food animal before harvest, it is necessary to give guidelines how long the growers should wait before the release of animals if they applied drugs. This period of necessary drug withholding, or withdrawal time (WT) is determined experimentally by feeding therapeutic doses in the laboratory. There are unique characteristics involved in WT determination using analytical tools in comparison with isotherms: (1) drug clearing time is highly dependent on water temperature and the time prolongs when the temperature falls (2) it is almost impossible to make the sick animals ingest the drug as we intend (3) most animals are schooling species in which all physiology and behavior are dependent each other. In the current presentation, discussions will be made for several cases in which MRL and WT were established in aquatic animals through experimental and available document studies.

Symposium : **ANAL1-4**
Recent Studies in Bioanalyses Using Non-human Subjects
Room 104 THU 16:30
Chair: Wonryeon Cho (Wonkwang University)

Molecular Genetic Study of Capsainoids Biosythetic Pathway

Byoung-Cheorl Kang

Department of Agriculture, Forestry and Bioresources, Seoul National University, Korea

Capsaicinoids are major ingredients in the spicy taste of peppers, and it is used not only as food but also as a medicine due to its effects of pain relief, anti-cancer, anti-inflammatory, fat reduction, and antioxidant. However, only a few structural genes controlling capsaicinoids biosynthesis have been found, requiring further genetic and biochemical research. In addition, the capsaicinoids content varies depending on the genetic resource, and the amount of capsaicinoids production varies greatly depending on the environment conditions. However, there are very few studies on genes that control the capsaicinoid content, and developing a variety with different capsaicinoids amount is challenging. To reveal the biosynthesis pathway of capsicinoids, our groups has been conducting studies to identify structural genes and various transcriptional factors of capsaicinoids biosynthesis using various genetic sources and genetic analysis methods. First, to identify the genes that control the biosynthesis of capsaicinoids, the pepper reference genome information is improved through assembly and precise annotation of the pepper genome. Subsequently, the candidate genes are selected using various gene identification methods such as BSA-seq and MutMap. When a candidate gene is obtained through genetic analysis, the correlation between the capsaicinoids content and gene expression is investigated after knockdown of the candidate genes using a virus-induced gene-silencing method to test the function of the genes. Using various genetic resources containing different capsaicinoid amount, RNA-seq and GC methods are used to study the correlation between candidate genes and the capsaicinoid precursors to reveal the mechanism of capsaicinoid biosynthesis and its regulation.

Symposium : **ANAL2-1**
Current Trends in Molecular Sensing Techniques for Bio and Environmental Analysis
Room 104 FRI 14:30
Chair: Youngsoo Kim (Yeungnam University)

Detection of hazardous materials in the Environment

Sung Ik Yang

Department of Applied Chemistry, Kyung Hee University, Korea

Various substances, including heavy metals, nanoparticles, microplastics, and molds, exist in the environment. These substances can potentially affect human health as well as various organisms in the environment. For example, Inorganic mercury salts are water-soluble and cause damage to kidneys. These detrimental effects of mercury exposure have provoked the increased interest in developing detection tools for mercury in environments. Mold detection, especially in indoor environments, is becoming increasingly important because molds pose a severe threat to human health. Although many methods for mold detection have been developed, including time-consuming culture-based detection, immunoassay, and DNA amplification-based detection, they are not suitable for rapid detection. In this talk, I plan to introduce the various detection methods for the various hazardous materials.

Symposium : **ANAL2-2**

Current Trends in Molecular Sensing Techniques for Bio and Environmental Analysis

Room 104 FRI 14:50

Chair: Youngsoo Kim (Yeungnam University)

Single entity electrochemistry for the detection of blood cells

Byung-Kwon Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Single entity electrochemistry (i.e., single particle collision, or nano-impact electrochemistry) on ultramicroelectrodes has been actively studied. This single particle collision method is a good way to analyze particle composition, size, concentration, diffusion coefficient, and behavior in solution. Recently, our group have studied some soft particles such as emulsions (water/oil and oil/water), bacteria, red blood cells and platelets by single entity electrochemistry. The current increase or decrease which occurs when the soft particles collide with the electrode surface were measured. These methods can be used as a fundamental technology to detect various types of biomaterials.

Symposium : **ANAL2-3**
Current Trends in Molecular Sensing Techniques for Bio and Environmental Analysis
Room 104 FRI 15:20
Chair: Youngsoo Kim (Yeungnam University)

Synthesis of Noble Metal Nanostructure Probes with Controlled Sizes and Shapes for Bioanalytical Applications

Jae-Seung Lee

Department of Materials Science and Engineering, Korea University, Korea

Noble metal nanoparticles exhibit a variety of unique chemical and physical properties, such as intense optical properties in UV-vis spectroscopy or surface-enhanced Raman scattering (SERS), catalytic properties, and easy fabrication of the surface nature using functional ligands. Such properties are strongly correlated with their morphology, which has brought a great deal of attention to the delicate design of nanostructures. Even though the synthetic strategies for controlling the shapes of monometallic nanomaterials such as gold (Au) and silver (Ag) are well-developed, limited advances have been made with bi- and trimetallic nanomaterials to date. To address these issues, we have developed a rapid one-pot room-temperature aqueous synthesis of highly monodisperse AgCl nanotemplates, which are successfully replicated into bi- and trimetallic nanomesh structures. The multimetallic nanostructures are small enough (~100 nm) to show intense surface-plasmon-absorption bands. The complex comprising semiconducting AgCl/metallic nanomesh replicas exhibit excellent plasmonic photocatalysis properties and intense surface-enhanced Raman scattering (SERS) properties in a single-particle. Their applications as nanoprobes for ultrahigh sensitive colorimetric detection are also demonstrated.

Symposium : **ANAL2-4**

Current Trends in Molecular Sensing Techniques for Bio and Environmental Analysis

Room 104 FRI 15:40

Chair: Youngsoo Kim (Yeungnam University)

Plasmonic biosensing with static nanogap or dynamic nanogap

Jeong-Wook Oh

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Plasmonic coupling enables to provide superior optical enhancement, which effect is significantly affected by the nanogap thickness. A narrower nanogap can confine the light in the nanogap and magnify the electromagnetic field, enhancing surface-enhanced Raman scattering (SERS). Thus, in terms of biosensors, the precise control of plasmonic nanogap thickness can improve the optical signal intensity to detect a low quantity of target molecules and provide dynamic information of binding events of biomolecules. Here, we developed DNA-modified Au nanostructures with 1-nm static nanogap, which was applied as highly sensitive SERS probes, and monitored DNA hybridization kinetics using dynamic plasmonic coupling with Au nanoparticles on the fluidic lipid layer.

Symposium : **ANAL2-5**

Current Trends in Molecular Sensing Techniques for Bio and Environmental Analysis

Room 104 FRI 16:00

Chair: Youngsoo Kim (Yeungnam University)

Toehold DNA probes-mediated analysis for simple, specific, and sensitive detections of pathogen DNA

Cheolam Hong

Department of Chemistry and Biochemistry, Yeungnam University, Korea

High specific and sensitive detection of specific DNA is important for the early diagnosis and effective treatment because its sequences are closely related to the cause and development of various diseases such cancer and genetic disorders. Presently, the most widely used analysis for detecting specific DNA is the quantitative real-time polymerase chain reaction (qRT-PCR), which can be sufficient to amplify very low abundance DNA to detectable levels by the rapid and repetitive heating and cooling cycles with specific enzymes. However, this analysis requires the expensive reagents, enzymes, and equipment, and complex and time-consuming steps. Therefore, achieving simple and low-cost detection of specific DNA still remains a considerable challenge. To this end, our research is to develop a variety of toehold DNA probes for simple, sequence-specific, and ultra-sensitive detection under the enzyme- and analytic instrument-free reactions at the room temperature. In this talk, we will introduce various strategies of the toehold DNA probes to detect specific DNA such cancer and pathogens.

Symposium : **LIFE1-1**
Diversity in Polymer Therapeutics
Room 105 THU 15:40
Chair: Chan Hyuk Kim (KAIST)

Therapeutic development using chemically modified asymmetric small interfering RNAs

Dong-ki Lee

Department of Chemistry, Sungkyunkwan University, Korea

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

Symposium : **LIFE1-2**
Diversity in Polymer Therapeutics
Room 105 THU 16:10
Chair: Chan Hyuk Kim (KAIST)

Bilirubin-derived nanomedicine as a novel therapeutic for intractable inflammatory diseases

Sangyong Jon

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

Despite the high potency of bilirubin (BR) as an endogenous anti-inflammatory compound, its clinical translation has been hampered because of its insolubility in water and potential toxicity on erythrocytes and immune cells. To overcome the critical issues, we attached polyethylene glycol (PEG) to BR, yielding PEGylated bilirubin (PEG-BR). The PEG-BR self-assembled into nanoscale particles with a size of approximately 110 nm, termed bilirubin nanoparticles (BRNPs). Unlike free BR, BRNPs are fairly water-dispersible and circulate much longer in blood, thus overcoming a critical issue associated with the clinical use of BR. Recently, we demonstrated that BRNPs had potent therapeutic efficacy in animal models of several inflammatory diseases, including inflammatory bowel disease, acute asthma and hepatic ischemic reperfusion injury. We also demonstrated that BRNPs can be used as a dual-stimulus (light and ROS)-responsive drug-delivery carrier, reflecting the fact that BR in NPs undergoes a switch in water solubility and degradation in response to these stimuli. In this talk, I will share with audience recent research progress on multiple biomedical applications of bilirubin-based nanomedicine and also discuss about its clinical translation potential as a therapeutic for intractable inflammatory diseases.

Symposium : **LIFE1-3**
Diversity in Polymer Therapeutics
Room 105 THU 16:40
Chair: Chan Hyuk Kim (KAIST)

Possibilities and Challenges in Antibody-Drug Conjugate Technology

Chul-Woong Chung

Legochem Biosciences, Inc., Korea

Antibody-Drug Conjugates (ADCs) have emerged as one of the fastest growing pharmaceutical class of drugs designed to harness the specificity of antibodies with the potency of small molecule therapeutics. Although it has suffered from several failures in clinical trials, it is proving to be a successful technology through technological advancement step by step. Currently, 10 ADCs have been approved for therapeutic use, and the clinical success of these ADCs have sparked clinical development of novel ADCs. Lessons learned during the past decade are now being used in the development of next-generation ADCs. LegoChem Biosciences(LCB) has developed a novel next-generation site-specific ADC platform with novel linker chemistry that improves stability of ADCs, effectively prevents premature drug release, efficiently facilitates the liberation of the drug at the targeted tumor cells and ultimately shows significant improved therapeutic index. In addition, this presentation highlights LCB's tumor-selective and ultra-potent DNA-crosslinking payload with superior efficacy and reduced toxicity.

Symposium : **LIFE1-4**
Diversity in Polymer Therapeutics
Room 105 THU 17:10
Chair: Chan Hyuk Kim (KAIST)

Development of novel anti-CD19 CAR T cells resistant to PD-1 and TIGIT-mediated immune suppression

Hyung Cheol Kim

R&D Center, Curocell Inc., Korea

Currently, several CD19-directed chimeric antigen receptor (CAR) T cell therapies are commercially available and have become an important option for patients with refractory or relapsed B-cell leukemia and lymphomas. However, not all patients benefit from this novel therapy due to various resistance mechanisms. Since the expression of immune checkpoint receptors (ICRs) can impair the effector function of CAR-T cells, we have developed a lentiviral vector system that can efficiently induce shRNA-based silencing of ICR gene while maintaining robust CAR expression. Using this system, we successfully generated PD-1-downregulated CD19 CAR-T, which showed enhanced anti-tumor activity against PDL-1 positive cancer cells compared to control CAR-Ts. Then, given the possibility of a compensatory upregulation of another ICR, we extended our platform to silence two ICR genes simultaneously, and found that PD-1 and TIGIT dual downregulation for CD19 CAR-T (OVIS^{TM} CD19 CAR-T) exhibited a unique synergistic anti-tumor activity in vitro and in vivo, and that downregulation of PD-1 enhances short-term effector function, while downregulation of TIGIT plays a role in maintaining a less-differentiated/exhausted state of CAR-T. For the development of OVIS^{TM} CD19 CAR-T as an investigational new drug, the efficacy, safety, and specificity of OVIS^{TM} CD19 CAR-T was evaluated through non-clinical studies. Overall, our results show that PD-1 and TIGIT dual downregulation strategy can provide an effective way to overcome the immune checkpoint-mediated immune suppression. The safety and efficacy of the OVIS^{TM} CD19 CAR-T (CRC01) is currently being evaluated via a clinical trial (ClinicalTrials.gov Identifier: NCT04836507).

Symposium : **LIFE2-1**
Structural Approaches to Understanding the Biological Function of Macromolecules
Room 105 FRI 09:00
Chair: Jungwook Kim (GIST)

Structural and Mechanistic Diversity of anti-CRISPR proteins for CRISPR Inhibition

Jeong-Yong Suh

Agricultural Biotechnology, Seoul National University, Korea

Clustered regularly interspaced short palindromic repeats (CRISPRs) and CRISPR-associated (Cas) proteins provide adaptive immunity for prokaryotes against invading phages and plasmids. Phages evolved anti-CRISPR (Acr) proteins to neutralize the host CRISPR–Cas immune system as a counter-defense mechanism. Acr proteins are generally small in size, and inhibit their host CRISPR-Cas proteins in a stoichiometric or enzymatic manner. Here, I introduce diverse structural and functional mechanisms of Acr proteins known to date, and describe our recent study on types II-A and II-C Acr proteins. AcrIIA4 binds to the target DNA recognition site of Cas9 to compete with DNA binding, whereas AcrIIA5 employs an intrinsically disordered region to interfere with the catalytically active conformation of Cas9. AcrIIC2 disrupts the guide RNA binding to Cas9, and AcrIIC3 inhibits Cas9 in an allosteric manner. New folds and functional mechanisms of Acr proteins will expand our knowledge on the evolutionary arms race between bacteria and phage, and also promise applications in the precision control of gene editing.

Symposium : **LIFE2-2**

Structural Approaches to Understanding the Biological Function of Macromolecules

Room 105 FRI 09:25

Chair: Jungwook Kim (GIST)

Structures of viral pyrimidine hydroxymethylases using X-ray free electron laser

Hyun Kyu Song

Division of Life Sciences, Korea University, Korea

The hydroxymethylation of pyrimidine bases plays a vital role in the phage DNA protection system inside the host bacteria. This modification is known to be catalyzed by the dCMP and dUMP hydroxymethylases (dCH and dUH) from bacteriophages. However, the detailed mechanism has not been understood clearly due to lack of structures in the complex with a reaction intermediate. We have applied the X-ray free electron laser (XFEL) technique to determine a high-resolution structure of dCH D179N mutant from T4 phage. Unexpectedly, we observed a bulky electron density for dTMP at the active site of the mutant that originated from the physiological host (i.e., E. coli). The bound dTMP mimicked the methylene intermediate from dCMP to 5'-hydroxymethyl-dCMP, and a critical water molecule for the final hydroxylation was convincingly identified. Furthermore, we also determined the structure of dUH from Salmonella phage ViI in apo and complex with dUMP using conventional X-ray as well as XFEL methods. This is the first structural report of dUH enzyme and provides information that contributes to understanding the specificity of pyrimidine bases. The comparison between dCH and dUH will be presented.

Symposium : **LIFE2-3**

Structural Approaches to Understanding the Biological Function of Macromolecules

Room 105 FRI 09:50

Chair: Jungwook Kim (GIST)

Cryo-EM structure of a mitochondrial calcium uniporter

Jiho Yoo

College of Phamacy, Chung-Ang University, Korea

Calcium transport plays an important role in regulating mitochondrial physiology and pathophysiology. The mitochondrial calcium uniporter (MCU) is a calcium-selective ion channel that is the primary mediator for calcium uptake into the mitochondrial matrix. Here, we present the cryo-electron microscopy structure of the full-length MCU from Neurospora crassa to an overall resolution of ~3.7 angstroms. Our structure reveals a tetrameric architecture, with the soluble and transmembrane domains adopting different symmetric arrangements within the channel. The conserved W-D-Φ-Φ-E-P-V-T-Y sequence motif of MCU pore forms a selectivity filter comprising two acidic rings separated by one helical turn along the central axis of the channel pore. The structure combined with mutagenesis gives insight into the basis of calcium recognition.

Symposium : **LIFE2-4**

Structural Approaches to Understanding the Biological Function of Macromolecules

Room 105 FRI 10:15

Chair: Jungwook Kim (GIST)

Understanding the mechanism of assembly and modifications of DNA high-order structure

Ji-Joon Song

Department of Life Science, KAIST, Korea

Abo1 is a conserved histone chaperone in fission yeast that contains a bromodomain and two AAA+ ATPase domains. Its human ortholog, ATAD2 has been implicated in various types of human cancers and holds potential as a therapeutic drug target. Despite evidence that Abo1 and its orthologs regulate nucleosome density and transcriptional activity in cells, the exact function of Abo1 is yet unknown. Moreover, structural studies of the Abo1 family are limited, thus hindering mechanistic understanding of these proteins. In this study, we show the first view of the overall architecture of the Abo1 family at 3.6Å by cryo-EM. We find that in the ATP state, Abo1 forms an asymmetric hexameric spiral that binds the histone H3 tail by a negatively charged pore and a hydrophobic tryptophan staircase. In contrast, Abo1 in the ADP or apo state assumes a symmetric, planar hexameric ring. These types of nucleotide-dependent structural changes are visualized in real-time by video AFM, and are shown to contribute to ATP-dependent histone deposition onto DNA in a single molecule fluorescence DNA curtain assay. Altogether, these findings reveal a novel mechanism for a histone chaperone, and serve as an initial step towards understanding the molecular process of nucleosome assembly

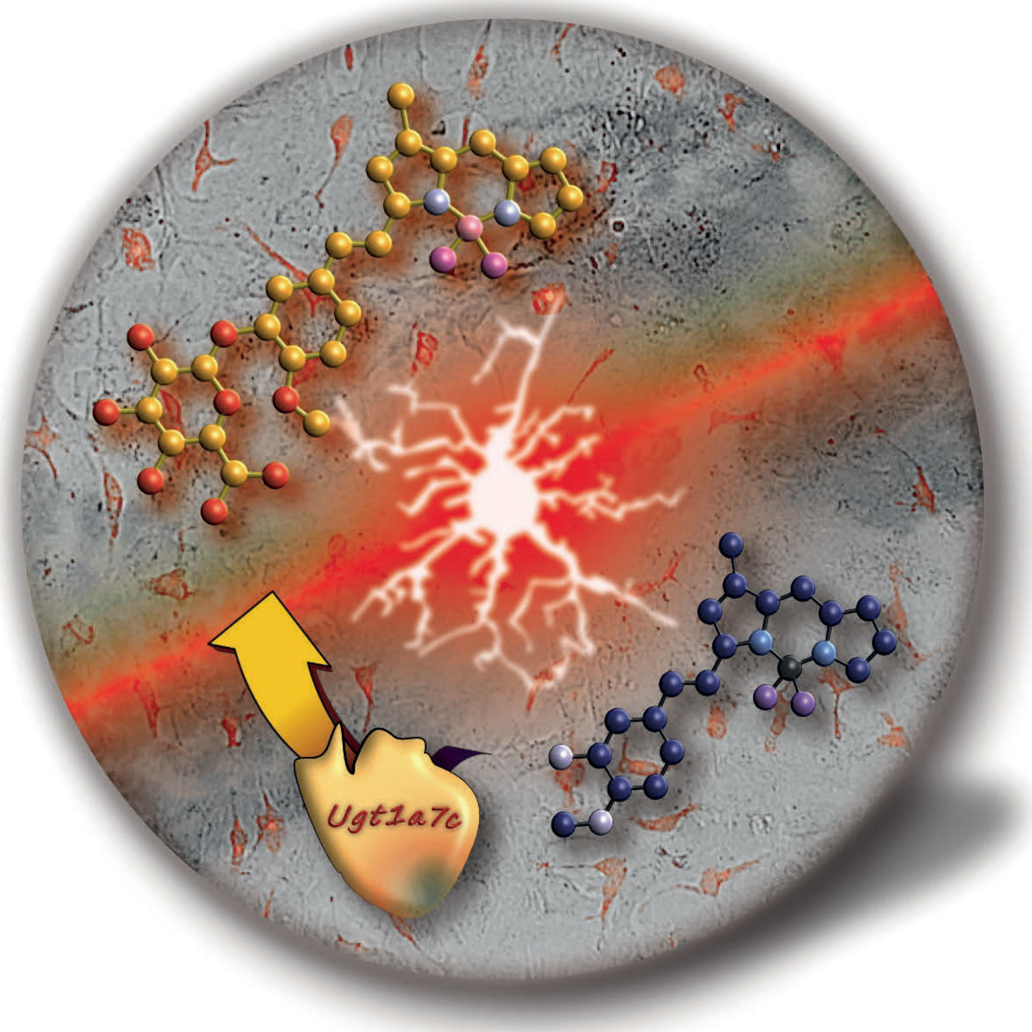
Symposium : **LIFE2-5**
Structural Approaches to Understanding the Biological Function of Macromolecules
Room 105 FRI 10:40
Chair: Jungwook Kim (GIST)

Metabolism Oriented Live-cell Distinction (MOLD) for immune cells

Young-Tae Chang

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

Distinctive imaging of each cell types in multicellular tissue is the most important first step to understand the complex cell community and control their regulation. The conventional approach of cell distinction is through binding biomarkers such as proteins and carbohydrates: Protein Oriented Live-cell Distinction (POLD) and Carbohydrate Oriented Live-cell Distinction (COLD). While relatively new approach of Gating Oriented Live-cell Distinction (GOLD) provides another possible route for cell study, the intrinsically complex nature of tissue requires further orthogonal strategy for higher dimension of cell discrimination. Here we report novel chemical biology approach of Metabolism Oriented Live-cell Distinction (MOLD) to enrich the toolboxes and strategy option. The design and mechanism elucidation will be presented with various immune cell discriminations, proposing new direction cell selective probe development. The multi-dimensional layer of cell distinction power will be the basis of analyzing extremely complex cell communities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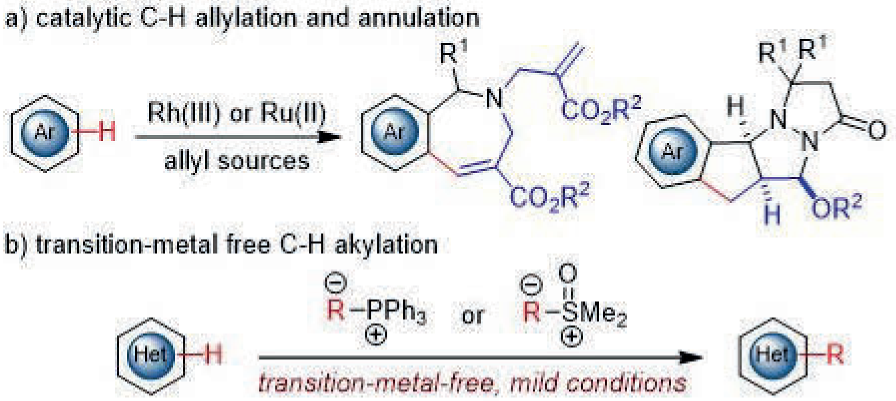
Award Lecture in Division : **ORGN1-1**
Current Trends in New Reactions and Methodology
Room 201 THU 15:40
Chair: Eun Joo Kang (Kyung Hee University)

C-H Allylation and Alkylation for the Construction and Functionalization of N-Heterocycles

In Su Kim

School of Pharmacy, Sungkyunkwan University, Korea

The C−H allylation and annulation with various π-unsaturated reactants has been recognized as a valuable strategy for the efficient construction of bioactive N-heterocyclic molecules (Review, ACS Catal 2017) Recently, our group disclosed the Rh(III)-catalyzed C−H allylation and in situ annulation reaction using Morita–Baylis–Hillman (MBH) adducts as allyl sources to afford 2-benzazepines (ACS Catal 2018), bridged benzoxazepines (OL 2018), and 2-naphthols (OCF 2018). Very recently, we found that allylic acetals as highly activated acrolein oxonium precursors have been also employed for C–H allylation reactions (ACIE 2019). Interestingly, allylic acetals are capable of olefin insertion into a ruthenacycle species to deliver the vinyl ether adducts, which further undergo [3+2] dipolar cycloaddition to afford synthetically and biologically valuable indenopyrazolopyrazolones.Beyond C−H allylation reactions, the direct C−H alkylation of N-heterocycles is an important transformation for the advancement of pharmaceuticals, agrochemicals, functional materials, and other chemical entities. Herein, we explored the unprecedented reductive alkylation of pyridine and quinoline-N-oxides using Wittig reagents as novel aromatic alkylation surrogates (ACIE 2018, OL 2019). In addition, we described the C2-selective C−H alkylation of heterocyclic N-oxides with sulfonium ylides (OL 2020). Moreover, we developed the C(sp2)–H alkylation of iminoamido heterocycles as nucleoside base analogues with sulfur ylides as alkylating agents under aqueous conditions (ACIE 2021). The applicability of the developed protocol is showcased by the late-stage alkylation and sequential transformations of complex drug molecules.


a) catalytic C-H allylation and annulation
Ar
H
Rh(III) or Ru(II)
allyl sources
R1
N
CO2R2
CO2R2
R1 R1
H
N
N
O
H
OR2
b) transition-metal free C-H akylation
Het
H
R
PPh3
or
O
SMe2
transition-metal-free, mild conditions

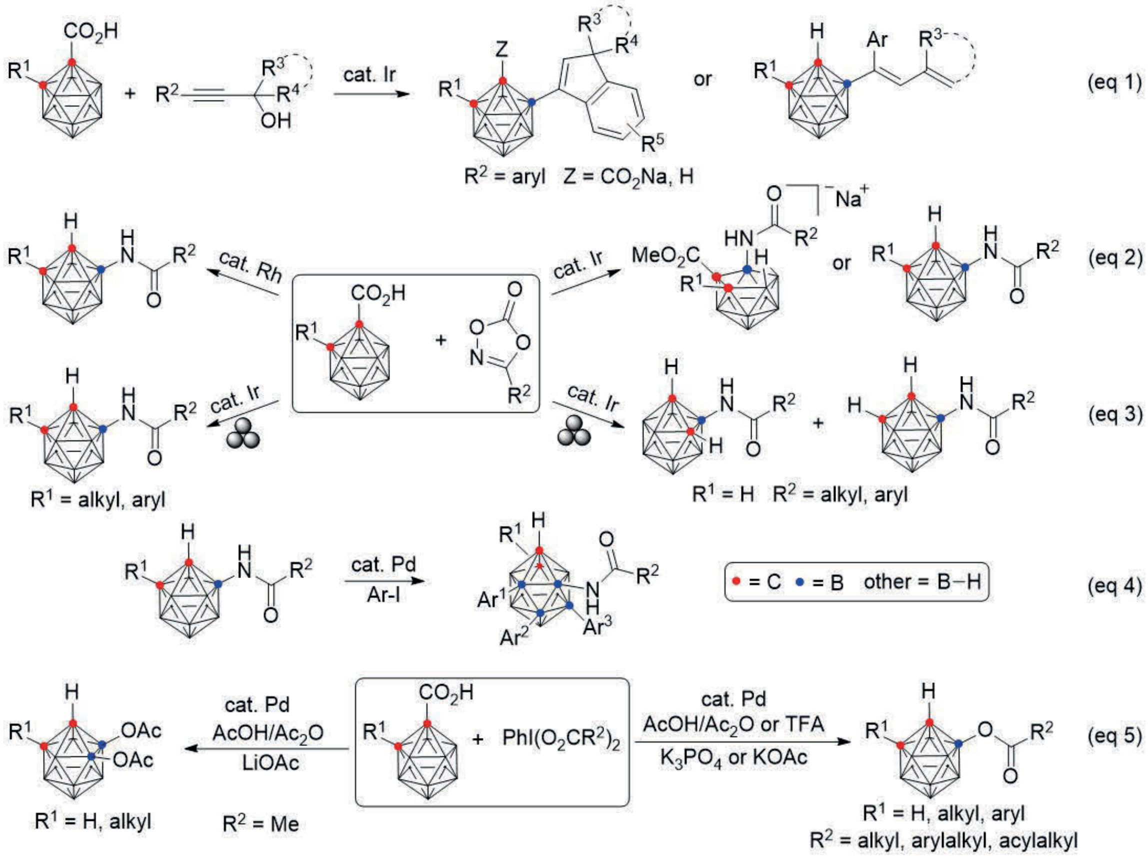
Symposium : **ORGN1-2**
Current Trends in New Reactions and Methodology
Room 201 THU 16:10
Chair: Won-jin Chung (GIST)

Functionalization of *o*-Carboranes

Phil Ho Lee

Department of Chemistry, Kangwon National University, Korea

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


CO2H
R1
+
R2
R3
R4
OH
cat. Ir
Z
R5
R2 = aryl Z = CO2Na, H
or
H
Ar
(eq 1)
cat. Rh
HN
R2
O
cat. Ir
MeO2C
O
Na+
or
(eq 2)
N
O
cat. Ir
(eq 3)
R1 = alkyl, aryl
R1 = H R2 = alkyl, aryl
cat. Pd
Ar-I
Ar1
Ar2
Ar3
● = C ● = B other = B–H
(eq 4)
OAc
cat. Pd
AcOH/Ac2O
LiOAc
PhI(O2CR2)2
cat. Pd
AcOH/Ac2O or TFA
K3PO4 or KOAc
(eq 5)
R1 = H, alkyl
R2 = Me
R1 = H, alkyl, aryl
R2 = alkyl, arylalkyl, acylalkyl

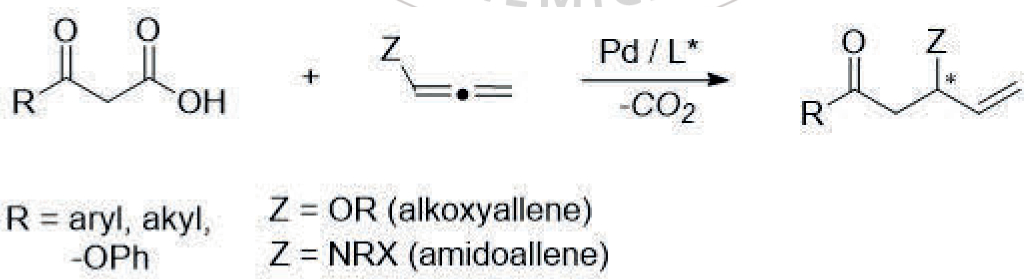
Symposium : **ORGN1-3**
Current Trends in New Reactions and Methodology
Room 201 THU 16:30
Chair: Won-jin Chung (GIST)

Pd-catalyzed Asymmetric Decarboxylative Addition of β-Keto Acids to Alkoxy- and Amidoallenes

Young Ho Rhee[*], **Sukhyun Lee, Dong-Jin Jang, Juyeol Lee**

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

Branch-selective asymmetric hydrofunctionalization of allene represents a fundamentally important synthetic transformation, because of its unique atom efficiency as well as the capability to generate a stereogenic center. In this context, we report here our recent results on the Pd-catalyzed decarboxylative addition of β-keto acids to heteroatom-substituted allenes such as alkoxy- and amidoallenes. The latter is particularly notable since (asymmetric) branch-selective hydrofunctionalization of amidoallene is rare.Through extensive mechanistic studies, the initial hydrocarboxylation of allene was established as the key event, which facilitates the subsequent asymmetric decarboxylative C-C bond formation. The reaction generates densely functionalized γ,δ-unsaturated ketones possessing heteroatom substituents at the β-position. The utility of the reaction was demonstrated highly flexible stereodivergent synthesis of cyclic ethers.



R = aryl, akyl,
-OPh

Z = OR (alkoxyallene)
Z = NRX (amidoallene)

Symposium : **ORGN1-4**
Current Trends in New Reactions and Methodology
Room 201 THU 16:50
Chair: Won-jin Chung (GIST)

Investigation of Regioselective C–H Functionalization of Heteroarene

Sungwoo Hong

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

The site-selective C–H bond functionalization of heteroarenes is highly desirable in the broad field of chemical research. Chemical methods to achieve this goal could have broad application potential in synthetic organic chemistry, considering the reduction in the number of synthetic steps and the abundance of inexpensive starting materials. The new catalytic synthetic methods allow us to perform the unprecedented disconnection of target molecules, affording innovative and imaginative synthetic strategies of so-called “privileged scaffolds”. Visible-light-induced site-selective heteroarylation of remote C(sp3)–H bonds has been accomplished through the design of a new methodology. The synthetic potential of pyridinium salts will be discussed as versatile pyridine surrogates to address various chemical transformations. In light of these benefits, our group leveraged the steric and electronic properties of the N-substituent of pyridinium salts to control the functionalization of pyridines. These new synthetic methods will function as competent tools directly utilized in cross-coupling reactions capable of connecting privileged building blocks, providing opportunities for the successful implementation of fragment-based drug design (FBDD), and eventually streamline drug discovery research.

Symposium : **ORGN1-5**
Current Trends in New Reactions and Methodology
Room 201 THU 17:10
Chair: Won-jin Chung (GIST)

A unified synthetic strategy to introduce heteroatoms via controlled functionalization of alkyl organometallic reagents

Hong Geun Lee

Department of Chemistry, Seoul National University, Korea

Based on systematic analyses, an integrated synthetic platform of C(sp3)-based organometallic compounds was established for the introduction of heteroatoms. The bond-forming strategy was shown to be highly effective for the functionalization of sp3-hybridized carbon atoms with significant steric hindrance. Moreover, virtually all the nonmetallic heteroatoms could be utilized as reaction partners, a property that has not been realized with previous approaches. The observed reactivity stems from the two consecutive single-electron oxidations of the substrate, which eventually generates an extremely reactive carbocation as the key intermediate. The detailed reaction profile could be elucidated through multifaceted mechanistic studies and the examination of the reaction kinetics.

Symposium : **ORGN2-1**

Current Trends in Medicinal and Process Chemistry

Room 201 FRI 09:00

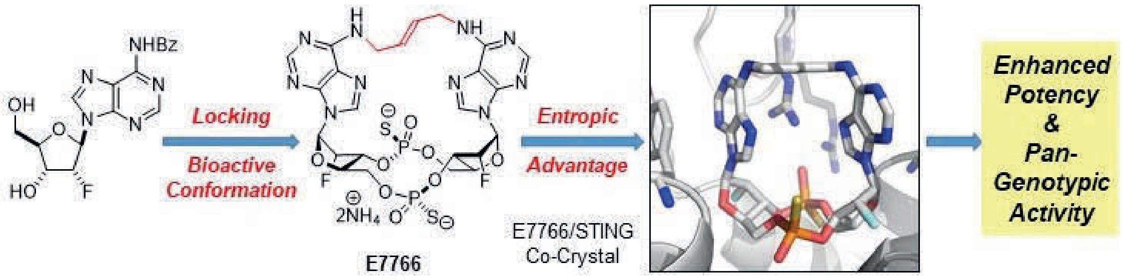
Chair: Hyejin Kim (KRICT)

Discovery of E7766, a Macrocycle-Bridged STING Agonist with Pan-Genotypic Activity

Dae-Shik Kim

Precision Chemistry, Eisai G2D2, United States

Stimulator of interferon genes (STING) is an emerging target for cancer immunotherapy. Modification of cyclic dinucleotides (CDNs), natural ligands for STING, is a main approach to generate drug candidates. Eisai's unique strategy, locking STING active CDN conformation, led to discovery of a novel class of STING agonists, macrocycle-bridged STING agonists (MBSAs). E7766, a representative MBSA, shows activity against four major STING variants and enhanced potency over a reference compound, and is in clinical trials. After initial ring closing metathesis (RCM) route for E7766, a stereoselective synthetic route has been developed for accessing new MBSA analogs and process development (ref. ChemMedChem 2021, 16, 1740–1743).



ChemMedChem **2021**, *16*, 1740–1743

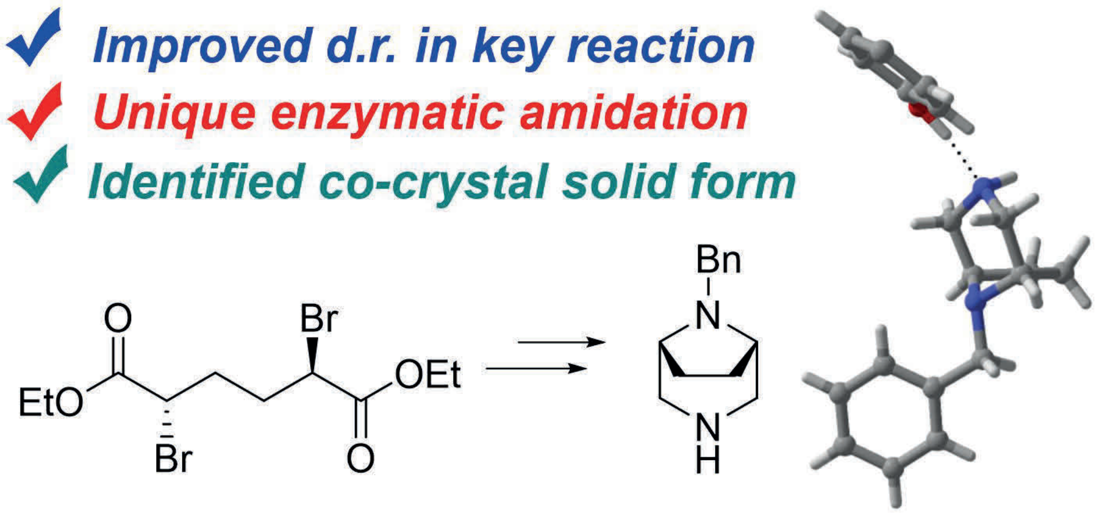
Symposium : **ORGN2-2**
Current Trends in Medicinal and Process Chemistry
Room 201 FRI 09:25
Chair: Hyejin Kim (KRICT)

Streamlined Synthesis of a Bicyclic Amine Moiety Using an Enzymatic Amidation and Identification of a Novel Solid Form

Taegyo Lee

Chemical Research and Development, Pfizer, United States

We describe a series of improvements to the synthesis of a 3,8-diazabicyclo[3.2.1]octane derivative that result in a reduced step count and higher overall efficiency compared to previously published syntheses. Our method includes optimization and mechanistic understanding of a key diastereoselective cyclization to achieve a >95:5 diastereomeric ratio, as well as demonstration of a unique enzyme-catalyzed amidation reaction using hexamethyldisilazane as both an ammonia source and scavenger. Finally, we identify a novel cocrystal solid form of the target compound that provides improved purity and material properties. Demonstration of the new chemistry to prepare >100 kg of the target compound serves to illustrate the robustness of the new process.



Symposium : **ORGN2-3**
Current Trends in Medicinal and Process Chemistry
Room 201 FRI 09:50
Chair: Hyejin Kim (KRICT)

Development of Biocatalytic Manufacturing Processes for an HIV agent Islatravirand a Covid-19 antiviral Molnupiravir

Jongrock Kong

Process Research & Development, Merck & Co., United States

Biocatalysis is increasingly important in the pharmaceutical industry for the development of cost-effective and eco-friendly drug manufacturing processes. Merck & Co., Inc., Kenilworth, NJ, USA Process Research & Development has a long history of biocatalysis innovation and continues to focus on applications of novel biocatalytic transformations for the synthesis of active pharmaceutical ingredients at all stages of development. This presentation will highlight two stories about development of biocatalytic processes for the synthesis of antiviral agents islatravir and a Covid-19 antiviral molnupiravir. The first part will include the discovery of an asymmetric synthetic route that utilized a biocatalytic desymmetrization for an expedient multi-kilogram synthesis of islatravir to enable first in human (FIH) clinical studies, as well as enzymatic cascade toward the development of a more cost-effective and innovative manufacturing route. In the second part, the rapid process development of the Covid-19 therapeutic molnupiravir will be presented, including an efficient selective 5’-acylation of ribose, a novel biocatalytic cascade featuring an engineered ribosyl-1-kinase and uridine phosphorylase and a direct conversion of amidic carbonyl in the uracil ring to the corresponding oxime.

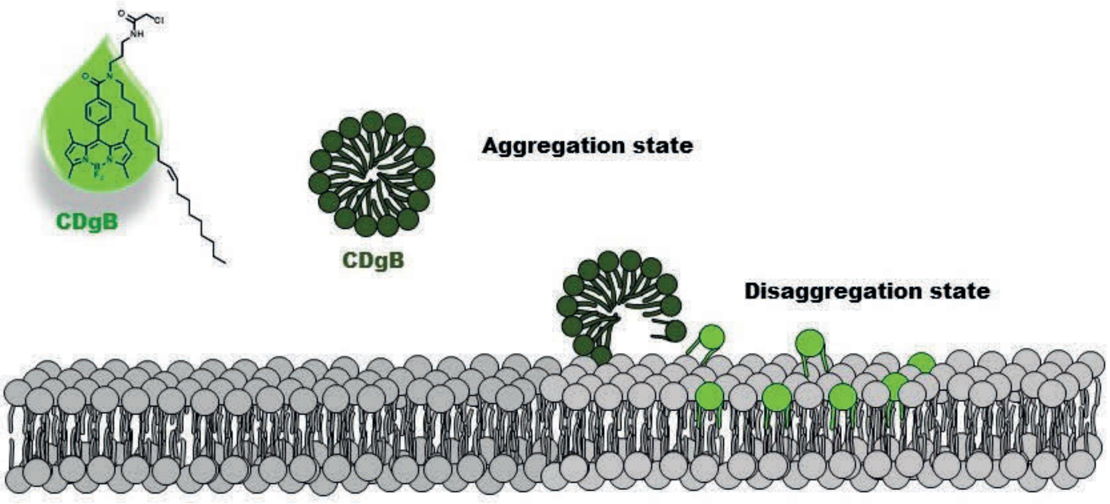
Symposium : **ORGN3-1**
Current Trends in Chemical Biology and Bioorganic Chemistry
Room 201 FRI 14:30
Chair: Jongmin Park (Kangwon National University)

New chemical approach for live cell distinction through lipid in cell membrane

Young-Tae Chang

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

Distinction of cell types in multicellular organism is the very basic first step to understand the complex cell community and manipulating their interactions. The conventional approach of cell distinction is through magic bullet molecule for specific biomarker in each cell. Proteins and carbohydrates have been the most popular binding targets for fluorescent probe. Here I report a new approach of cell distinction through the lipid composition on plasma membrane. In addition to Protein Oriented Live-cell Distinction (POLD) and Carbohydrate Oriented Live-cell Distinction (COLD), Lipid Oriented Live-cell Distinction (LOLD) provides totally different dimension of cell discriminating power for analyzing complex cell system, such as immune system. The first B cell selective probe CDgB and LOLD mechanism, elucidated from T and B lymphocyte distinction campaign, has been applied to the origin analysis of immune cell maturation.



Symposium : **ORGN3-2**
Current Trends in Chemical Biology and Bioorganic Chemistry
Room 201 FRI 14:55
Chair: Jongmin Park (Kangwon National University)

Effect of molecular chameleonicity on the membrane permeability of macrocyclic peptide cyclosporin O derivatives

Jiwon Seo

Chemistry, Gwangju Institute of Science and Technology, Korea

Macrocyclic peptides have emerged as a promising modality to inhibit intracellular protein-protein interactions (PPIs). Membrane permeability is a key factor to the pharmaceutical utility of the macrocyclic peptides providing access to the intracellular target and favorable pharmacokinetic profile. Along with various physico-chemical profiles, a ‘chameleonic’ ability to change their conformation to expose polar groups in aqueous solution, but bury them when traversing lipid membranes, is considered as a unique property of certain oral macrocyclic drugs (e.g., cyclosporin A or CsA). To facilitate the usage of this class of macrocycles, a molecular scaffold with well-established structure-property relationship (SPR) is desirable. Here, we adopted cyclosporin O (CsO) as a synthetically accessible scaffold, prepared a library of CsO derivatives, and evaluated their structural characteristics and membrane permeability. Their conformations were characterized by NMR spectroscopy and calculated via molecular simulations with NMR constraints. In a lipophilic environment, CsA and CsO derivatives showed closed conformations, but in polar media, CsO derivatives exhibited a varying degree of chameleonicity depending on their side chain substitutions. Some of the CsO derivatives showed membrane permeability greater than CsA, as determined by the parallel artificial membrane permeability (PAMPA) and Caco-2 assay, and general structural aspect for greater chameleonicity and membrane permeability will be discussed. Our study helps in the understanding of CsO, a macrocyclic peptide less explored than CsA but with more potential for diversity generation, which has led to designable macrocyclic peptides with desirable permeability and biological functions.

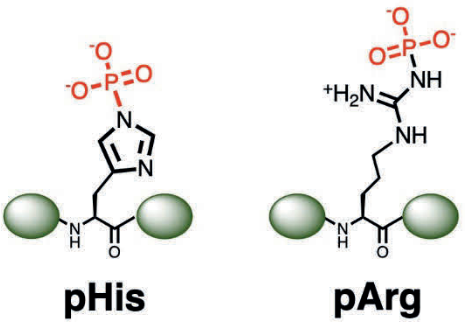
Symposium : **ORGN3-3**
Current Trends in Chemical Biology and Bioorganic Chemistry
Room 201 FRI 15:20
Chair: Jongmin Park (Kangwon National University)

Chemical Toolbox for Studying Histidine and Arginine Phosphorylation

Jung-Min Kee

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

Despite the well-recognized biological importance of protein phosphorylation, non-conventional forms of phosphorylation on histidine and arginine residues have evaded our attention and scrutiny for a long time. This lack of knowledge stems from the inherent chemical instability of phosphohistidine (pHis) and phosphoarginine (pArg), which makes the analysis of these phosphorylations notoriously challenging. Here we present our recent progress in developing novel tools, focusing on fluorescent sensors, to tackle these historically elusive protein modifications.



- ☐ Chemically unstable. Hard to study
- ☐ Novel chemical tools
  - ✓ Fluorescent sensors
  - ✓ Simple enzyme activity assays

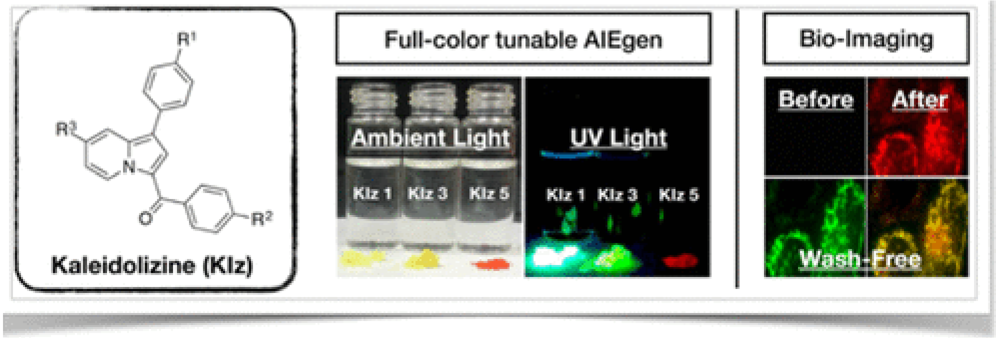
Symposium : **ORGN3-4**
Current Trends in Chemical Biology and Bioorganic Chemistry
Room 201 FRI 15:45
Chair: Jongmin Park (Kangwon National University)

Aggregation-Induced Emission Luminogen for Bioimaging Based on an Indolizine Molecular Framework

Eunha Kim

Department of Molecular Science and Technology, Ajou University, Korea

By taking advantage of a unique mechanism of aggregation-induced emission (AIE) phenomena, AIE luminogens (AIEgens) have been provided as a solution to overcome the limitations of conventional fluorophores bearing the feature of aggregation-caused quenching (ACQ) phenomena. Especially, AIEgens paved the way to develop fluorogenic probes ideal for fluorescent imaging in live cell conditions. Despite the high demand for discovery of new AIEgens, it is still challenging to find a versatile molecular platform to generate diverse AIEgens. Herein, we report a new colorful molecular framework, Kaleidolizine (KIz), as a molecular platform for AIEgen generation. The KIz system allows systematic tuning of the emission wavelength from 455 to 564 nm via perturbation of the electron density of substituents on the indolizine core. Increasing the water fraction of the KIz solution in the THF/water mixture induces the fluorescence intensity increase up to 120-fold. Crystal structure analysis, computational calculations, and solvatochromism studies suggest that a synergistic effect between the intramolecular charge transfer and restriction of intramolecular rotation acts as the AIE mechanism in the KIz system. Conjugation of the triphenylphosphonium moiety to KIz allows successful development of triphenylphosphonium (TPP)-KIz for real-time bioimaging of innate mitochondria in live cells, thereby revealing the potential of KIz as a versatile molecular platform to generate fluorogenic probes based on AIE phenomena. We do believe the KIz system could serve as a new, reliable, and generally applicable molecular platform to develop various AIEgens having desired photophysical properties along with an excellent signal-to-noise ratio and with experimental convenience especially for fluorogenic live cell imaging.


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

Symposium : **MEDI-1**

The Cutting Edge of Medicinal Chemistry

Room 106 THU 15:40

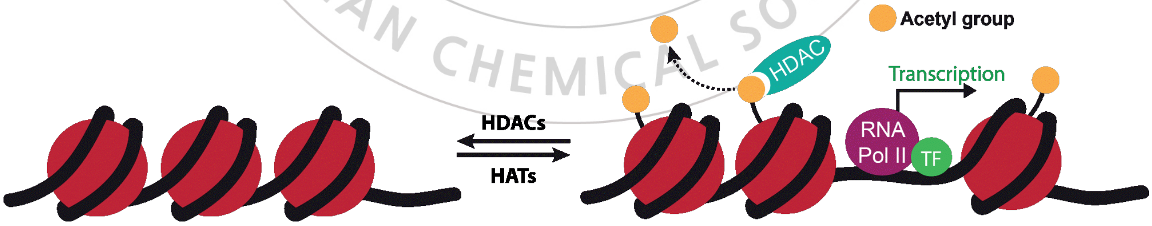
Chair: Kwan-Young Jung (KRICT)

Targeting Epigenetic Regulator HDAC Enzymes in Cancer

Young Ho Seo

College of Pharmacy, Keimyung University, Korea

Over the last two decades, numerous cancer drugs have been discovered as “targeted cancer drugs” to specifically kill cancerous cells while leaving healthy cells unharmed. Despite the robust efficacy of the targeted drugs, the ‘one target, one disease’ approach is being challenged by the occurrence of drug resistance. Cancer cells are intrinsically heterogeneous and tend to result from multiple molecular abnormalities. Therefore, pinpointing a single target is unlikely to eradicate cancer cells, which often find ways to compensate for the blockage of the protein by amplifying alternative signals or mutating targeted proteins. Therefore, to elucidate a drug simultaneously to attack multiple targets has been emerged as a new paradigm to overcome the drug resistance in cancer research. Here, we present our effort to develop therapeutic agents selectively to disrupt HDAC epigenetic regulators in cancer.



Symposium : **MEDI-2**
The Cutting Edge of Medicinal Chemistry
Room 106 THU 16:10
Chair: Kwan-Young Jung (KRICT)

Discovery of Bioactive Molecules from Bead-displayed Combinatorial Libraries

Hongchan An

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

The development of faster and less expensive ways to find bioactive chemicals remains a high priority in medicinal chemistry. One alternative to traditional high-throughput screening (HTS) is the preparation and screening of one bead one compound (OBOC) libraries. However, peptoids (oligomers of N-alkylated glycine units) widely used in OBOC libraries bind to proteins with modest affinity in most cases. This talk describes the chemical library construction with stiffer oligomers named PICCOs (Peptoid-Inspired Conformationally Constrained Oligomers) including VBAAs (Vinylogous Beta Amino Acids). Recent technology to encode the synthesis history of each individual bead using DNA will be discussed as well.

Symposium : **MEDI-3**
The Cutting Edge of Medicinal Chemistry
Room 106 THU 16:40
Chair: Kwan-Young Jung (KRICT)

Development of HDAC Inhibitors for Treatment of Inflammatory Bowel Disease

Jonghoon Kim

Department of Chemistry, Soongsil University, Korea

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

Symposium : **MEDI-4**
The Cutting Edge of Medicinal Chemistry
Room 106 THU 17:10
Chair: Kwan-Young Jung (KRICT)

Discovery of peripherally acting agents for metabolic disease

Jin hee Ahn

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

We seek to discover new small molecule agents that act upon peripheral tissue for metabolic disease including NASH. When a peripheral tissue-targeting compound unnecessarily penetrates BBB, CNS side effects can be caused. Therefore, discovering small molecules that do not penetrate BBB is expected to be advantageous for both drug discovery and academic study. In this presentation, we would like to share what we have studied.

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

Synthesis and Their Application of Nano-structured Chiral Materials

Room 107 THU 17:00

Chair: Jongnam Park (UNIST)

Diverse control of TiO_2-based nanostructures and their photoelectronic applications

Wan-In Lee

Department of Chemistry, Inha University, Korea

Titanium dioxide (TiO_2) is a wide band gap semiconductor that attracts extensive attention and has widely been investigated for various purposes, due to its unique electrical, optical, and physicochemical properties. Tailoring of TiO_2 nanostructures with large surface area, high crystallinity, and controlled morphology and porosity would be a crucial task to diversify their applications such as solar cells, photocatalysts, sensors, electrochromic devices, batteries, micro-machines, and others. In the present work, TiO_2-based nanostructures in various shapes and sizes have been selectively synthesized and applied to various mesoscopic solar cells and photocatalysis. TiO_2 nanoparticles (NPs), nanoporous spheres (SPs), hollow microspheres (HSs), nanorods (NRs), and microtubes (MTs) have been successfully tailored by wet-chemical route, and their formation mechanisms are systematically investigated and discussed. That is, TiO_2 NPs in the range of 5–70 nm, NRs of 50–150 nm, SPs of 100–1,000 nm, and unique HSs and MTs were selectively synthesized and utilized as electron transporting materials of various mesoscopic solar cells. Particularly, nanoporous SPs are a promising material to tailor pore structures of TiO_2 layer caused by their dual pores of wide external and narrow internal pores. We successfully controlled the diameters of SPs as well as their internal pore sizes and demonstrated that SPs are quite an ideal building block to construct effective TiO_2 architectures for dye-sensitized solar cells (DSSCs), quantum dot sensitized solar cells (QDSSCs), perovskite solar cells (PSCs). It has also been found that nanoporous SPs are effective for designing efficient photocatalysts due to their high surface area with dual pore structures and long-range structural interconnectivity facilitating the charge separation of photoexcited electron/hole pairs.

Symposium : **MAT1-1**
Synthesis and Their Application of Nano-structured Chiral Materials
Room 107 THU 15:40
Chair: Jongnam Park (UNIST)

How Chirality of Light Can Be Transmitted into Supramolecular Polymers

Myungeun Seo

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

Homochirality is one of the most unique features in life. Since the racemic state should dominate in the prebiotic stage, origin of homochirality has been sought, in conjunction with evolution of life, that could lead to breaking of the mirror symmetry. Circularly polarized light (CPL) has been considered one of possible deterministic origins that inherently contain chiral information. Here we discuss how the chiral information encoded in CPL can be transmitted into supramolecular polymers beyond molecules, and further compete with accumulating molecular chirality to dictate the overall supramolecular helical sense. We will show that supramolecular chirality can be determined by an interplay of molecular chirality with CPL in constructive and destructive manners. Our results will provide insight on design of hierarchical chiral materials with orthogonal chirality control at different levels.

Symposium : **MAT1-2**
Synthesis and Their Application of Nano-structured Chiral Materials
Room 107 THU 16:00
Chair: Jongnam Park (UNIST)

Near-infrared Single-walled Carbon Nanotubes for Dynamic Neurochemical Imaging

Sanghwa Jeong

School of Biomedical Convergence Engineering, Pusan National University, Korea

Release and reuptake of neuromodulator serotonin is central to mood regulation and neuropsychiatric disorders, whereby imaging serotonin is of fundamental importance to study the serotonin signaling system. Recently, I present a reversible near-infrared optical probe for serotonin that reports physiologically-relevant serotonin concentrations on relevant spatiotemporal scales, and is compatible with pharmacological tests. Synthetic molecular recognition for serotonin was conferred by evolving molecular recognition between single stranded DNA (ssDNA) and single-walled carbon nanotube (SWNT). To do so, we developed a high-throughput screening platform for evolution of serotonin molecular selectivity, in which systematic evolution of ligands by exponential enrichment is implemented on carbon nanotube surfaces, a process we've termed SELEC. Our results suggest evolution of nanosensors could be generically implemented to rapidly develop other neuromodulator probes, and that these probes can image neuromodulator dynamics at spatiotemporal scales compatible with endogenous neuromodulation.

Symposium : **MAT1-3**
Synthesis and Their Application of Nano-structured Chiral Materials
Room 107 THU 16:20
Chair: Jongnam Park (UNIST)

Multiscale Inorganic Chiral Structures and Their Applications

Jihyeon Yeom

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

Inorganic materials possess impactful properties – e.g. optical, magnetic, and mechanical – due to the dense electron clouds, strong dipole moments, etc. Providing chirality to such inorganic materials in multiscale brings numerous unique properties. For example, when transition metal elements are incorporated in atomic chirality, due to the strong magnetic transition dipole moments, the optical activity of the system is amplified 1000 times and optical modulation is enabled in a very mild condition. By designing the chirality of ceramic materials from atomic- to micro-level, the optical activity from UV to SWIR can be obtained. The synthesis and analysis of such multiscale chiral inorganic materials are challenging. However, we can achieve it by controlling over chirality transfer from enantiomers or circularly polarized photons to matter. This talk will cover strategies of synthesis, analysis, and applications of atomic-, nano-, and micro- chiral inorganic materials.

Symposium : **MAT1-4**
Synthesis and Their Application of Nano-structured Chiral Materials
Room 107 THU 16:40
Chair: Jongnam Park (UNIST)

Peptide Induced Chirality in Single Gold Nanoparticle

Ki Tae Nam

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

Chiral structure controlled at nanoscale provides a new route to achieve intriguing optical properties such as polarization control and negative refractive index. However, asymmetric structure control with nanometer precision is difficult to accomplish due to limited resolution and complex processes of conventional methods. In this regards, utilizing chirality transfer occurring at organic-inorganic materials offers viable route to overcome these limitations. Previously we developed a unique synthesis strategy that characteristic of molecule is transferred to gold nanoparticle morphology. Based on the system, here, we demonstrated novel chiral gold nanostructures exploiting chirality transfer between peptide and high-Miller-index gold surfaces. Enantioselective adsorption of peptides results in unequal development of nanoparticle surface and this asymmetric evolution leads to highly twisted chiral element in single nanoparticle making unprecedented 432 helicoid morphology. The synthesized helicoid nanoparticle showed strong optical activity (dissymmetry factor of 0.2 at 622 nm) which was substantiated by distinct transmittance color change of helicoid solution under polarized light. Modulation of peptide recognition and crystal growth enabled diverse morphological evolution and the structural alterations provided tailored optical response, such as optical activity, handedness, and resonance wavelength. We believe that our peptide directed synthesis strategy offers a truly new paradigm in chiral metamaterial fabrication and will be beneficial in the rational design of chiral nanostructures for use in novel applications.

Award Lecture in Division : **MAT2-5**

Advanced Electrode Materials for Next-generation Batteries

Room 107 FRI 10:30

Chair: Hye Ryung Byon (KAIST)

Anionic and Cationic Clays as Building Blocks for Biomedical Materials

Jae-Min Oh

Department of Energy and Materials Engineering, Dongguk University, Korea

Clays can be chemical defined as 2-dimensional materials having metal oxide or hydroxide framework. They are abundant in nature with a variety of composition and chemical properties such as ion exchange capacity, catalytic property, biological activity and etc. Researchers have developed synthetic procedures for artificial clays and they have succeeded in controlling physical properties of artificial clays resulting in nanostructure clay materials. In this contribution, I am going to show several examples of natural or artificial clays for biomedical applications including drug delivery, diagnostics, biomedical products and etc. Most of clay materials were synthesized to have intended physical and chemical properties. Then, the materials were modified in various topologies according to the intended application: intercalation of drug molecules between layers for drug reservoir, surface modification with small molecules for cancer cell targeting property, lattice incorporation of certain ion for tracing application, formulation with organic moieties for further applications etc.

Symposium : **MAT2-1**
Advanced Electrode Materials for Next-generation Batteries
Room 107 FRI 09:10
Chair: Hye Ryung Byon (KAIST)

Molecular Layer Deposition of Li-ion Conducting "Lithicone" Film and its Application in Solid-State Batteries

Minjeong Shin

Department of Chemistry and Energy, Sungshin Women's University, Korea

Atomic layer deposition (ALD), and its organic equivalent molecular layer deposition (MLD), are promising thin film deposition techniques widely used in lithium battery applications. Among the various ALD/MLD films, Li-ion conducting films are of special interest due to their potential to be used as solid electrolytes or interfacial coatings in which facile ion transport is achieved. Several Li-ion conducting ALD films have been developed to date, however, research efforts to develop Li-conducting films prepared via MLD have been limited.The development of Li-containing films ("lithicone") via MLD is demonstrated, using lithium tert-butoxide (LiOtBu) as a lithium precursor and ethylene glycol (EG) as an organic linker. In situ quartz-crystal microbalance and spectroscopic ellipsometry were used to evaluate the lithicone MLD process. In addition, a suite of characterization techniques including X-ray photoelectron spectroscopy and atomic force microscopy were used to evaluate film growth characteristics and bonding environment of the film. Electrochemical impedance spectroscopy measurements show that annealed lithicone films exhibit room temperature ionic conductivity of $3.6–5 \times 10^{-8}$ S/cm with an activation energy of ~0.6 eV. Mechanical bending tests reveal that the lithicone MLD film exhibits superior mechanical properties in comparison to the ALD film.When applied at Li metal solid-state battery interfaces, lithicone coating expanded the stability voltage window compared to the control cell by forming favorable passivation layer to prevent solid electrolyte degradation. The lithicone MLD film provides a pathway to further develop Li-ion conducting materials for future battery applications.

Symposium : **MAT2-2**

Advanced Electrode Materials for Next-generation Batteries

Room 107 FRI 09:30

Chair: Hye Ryung Byon (KAIST)

Layered Double Hydroxides as High Performance Cathode Materials for Aqueous Rechargeable Batteries

Ji Hoon Lee

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

The increasing demand for lithium-ion batteries (LIBs) that are cheap and resistant to fire hazards promotes the research of aqueous rechargeable batteries (ARBs) as one of the promising alternatives. In spite of a great number of materials pool available in LIBs, different classes of electrolytes (i.e., non-aqueous and aqueous) would require entirely different approaches in developing electrode materials and corresponding operating conditions, which mainly originates from the markedly unstable electrode-electrolyte interface.Inspired by the presence of hydrated compounds founds near ponds, lakes, and sea, my efforts have explored hydrated compounds as ARB electrodes. In this talk, I will introduce my recent approaches in constructing ARBs using LDHs. LDHs are featured by their intercalated species located in their interlayer galleries such as anions and crystal water molecules. The detailed structure evolution of LDHs, revealed by in-situ X-ray characterization, would be mainly discussed.

Symposium : **MAT2-3**
Advanced Electrode Materials for Next-generation Batteries
Room 107 FRI 09:50
Chair: Hye Ryung Byon (KAIST)

Chemical prelithiation strategy preventing irreversible lithium loss in high capacity anodes

Minah Lee

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

The anode's initial Coulombic efficiency (ICE) is a crucial factor dictating the energy density of a practical Li-ion battery. Prelithiation has been considered an effective strategy to compensate for the irreversible lithium loss and thereby increasing ICE. However, most prelithiation methods reported so far utilize Li metal powder or molten Li, which cause safety issues and require high manufacturing costs. Solution–based chemical prelithiation using a reductive chemical promises unparalleled reaction homogeneity and simplicity. However, the chemicals applied so far cannot dope active Li in Si–based anodes but merely form solid–electrolyte interphases, leading to only partial mitigation of the cycle irreversibility. Herein, we show that molecularly engineered Li–arene complexes with sufficiently low redox potentials drive active Li accommodation in Si–based anodes to provide an ideal Li content in a full cell. [1] Fine control over the prelithiation degree and spatial uniformity of active Li throughout the electrodes is achieved by managing immersion time and temperature, promising both fidelity and low cost for large–scale integration. We further investigate a solvation rule to direct the Li+ intercalation mechanism of graphite-blend anodes, the most practical candidate for high-capacity anodes. [2] Combined spectroscopy and DFT calculations reveal that in weakly solvating solutions, free solvated-ion formation is inhibited during Li+ desolvation, thereby mitigating solvated-ion intercalation into graphite and allowing stable prelithiation of the blend.[References]1. J. Hong* and M. Lee* et al., Angewandte Chemie Int. Ed. 59, 14473 (202) 2. J. Hong* and M. Lee* et al., Journal of the American Chemical Society. 143, 9169 (2021)

Symposium : **MAT2-4**
Advanced Electrode Materials for Next-generation Batteries
Room 107 FRI 10:10
Chair: Hye Ryung Byon (KAIST)

Exploration of cathode materials for emerging calcium-ion batteries

Seung-Tae Hong

Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea

Calcium-ion batteries (CIBs) represent a promising alternative to the current lithium-ion batteries. Environmental friendliness, reliability, safety, and plentiful sources could be typical advantages of calcium over lithium. Calcium ions can transfer two electrons per ion. Thus, in principle, the capacity of a host material can double due to the divalency of calcium, provided the host material can release and accept the transferred electrons. The redox potential of calcium is close to that of lithium, enabling a high cell voltage. The larger ionic radius of calcium (1.0 Å) compared to those of other divalent ions (0.60–0.74 Å) could be advantageous for the diffusion in the host materials and the electrolytes due to the lower effective intercalant-ion charge density.Recent discoveries of reversible plating or alloying of calcium provoked considerable interest in calcium-based rechargeable batteries. Theoretical calculations also anticipate the development of positive materials. Nonetheless, only a few cathode materials have been reported so far, only to exhibit low energy-storage capability and poor cyclability. In this talk, the synthesis, structural and electrochemical properties of new cathode materials for nonaqueous CIBs will be presented, which were recently developed in our group. Some examples include NASICON-type $NaV_2(PO_4)_3$, $FeV_3O_9{\cdot}1.2H_2O$, $Ca_{0.13}MoO_3{\cdot}(H_2O)_{0.41}$, $K_{0.5}V_2O_5$, and $Ag_{0.33}V_2O_5$. These stimulating discoveries will lead to the development of new strategies for obtaining high energy density CIBs beyond LIBs.

Symposium : **MAT3-1**
Advanced Characterization in Materials Chemistry
Room 107 FRI 14:30
Chair: Jungwon Park (Seoul National University)

Operando microscopy to provide significant insights in battery chemistry

Hyun-Wook Lee

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

Operando analyses have provided several breakthroughs in the construction of high-performance materials and devices, including energy storage systems. However, despite the advances in electrode engineering, the formidable issues of lithium intercalation and deintercalation kinetics cannot be investigated via planar observations. In situ optical and transmission electron microscopy (OM and TEM) on lithium-ion batteries has offered diverse opportunities for monitoring the dynamic processes of electrodes during electrochemical reaction at both spatial and temporal resolution.In this talk, I will introduce side-view operando OM and TEM studies on anodes, for example graphite, silicon, and lithium metal that suffer lithium plating by overpotential, anomalous volumetric changes, fracture, or dendritic formation during lithiation process. Since the graphite color varies according to the optical energy gap during lithiation and delithiation, we could study the corresponding charge/discharge kinetics; in addition, our cell configuration uses liquid electrolytes similarly to commercial cells, allowing practical applications. Furthermore, this side-view observation has showed that microscale spatial variations in rate and composition control the insertion and desertion, revealing the kinetics through the whole electrode. The results of this study could enhance the fundamental understanding of the kinetics of battery materials.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Symposium : **MAT3-2**
Advanced Characterization in Materials Chemistry
Room 107 FRI 14:50
Chair: Jungwon Park (Seoul National University)

Characterization of ultrasmall nanoparticles using liquid-phase TEM and mass spectrometry

Byung Hyo Kim

Department of Organic Materials and Fiber Engineering, Soongsil University, Korea

Ultrasmall nanoparticles with a size range from 1 to 3 nm are hard to characterize by using conventional instruments because of its small-sized nature. Here, we present reliable methods for determining the size and structure of nanoparticles using mass spectrometry and liquid-phase TEM. First, we developed a liquid-phase TEM-based atomic structure characterization method. TEM images with different projection directions of ultrasmall metal nanoparticles can be obtained using liquid-phase TEM because nanoparticles rotate freely in liquid phase. The abundant TEM images from one nanoparticles were reconstructed to 3D structures with atomic precision. We obtained atomic maps of eight different nanoparticles and they show critical size and structural difference. Second, we developed mass spectrometry-based size characterization method. Matrix-assisted laser desorption/ionization time of flight (MALDI-TOF) mass spectrometer is appropriate for ultrasmall oxide nanoparticles because MALDI is one of the most soft ionization method and TOF covers theoretically unlimited detection range. We successfully obtained mass spectra of nanoparticles and convert the mass spectra to the size distribution using mass to convert equation we derived.

Symposium : **MAT3-3**

Advanced Characterization in Materials Chemistry

Room 107 FRI 15:10

Chair: Jungwon Park (Seoul National University)

Surfactant-free Synthesis of Nanoparticles via Discrete Single Entity Electrolysis of Aqueous Nanodroplets

Hyun Seo Ahn

Department of Chemistry, Yonsei University, Korea

An electrochemical synthetic strategy toward nanoparticles of various stoichiometries has been developed. This technique results in size and composition controlled nanoparticles that are directly anchored on an electrode and fully surfactant-free. Such strategy is expected to find broad appeal in the preparation of next generation electro- and photoelectro- catalysts in artificial photosynthesis.

Symposium : **MAT3-4**
Advanced Characterization in Materials Chemistry
Room 107 FRI 15:30
Chair: Byung Hyo Kim (Soongsil University)

Electrochemical and Chemical Pt Dissolution During Electrocatalysis

Chang Hyuck Choi

Gwangju Institute of Science and Technology, Korea

Electrochemical energy conversion has been perceived as one of the promising strategies to pursue a sustainable energy society. In this new energy scenario, electrocatalysts become the core technology, enabling efficient energy conversion between chemicals and electricity. For the successful implementation of electrocatalysts in real devices, their durable operation and promising initial activity are highly required. Over the last decades, considerable efforts have been made to improve their catalytic performance (e.g., doping, alloying, morphology engineering, etc.), successfully leading to remarkable advances in their initial activity, thereby showing potential feasibility for practical applications. However, our understanding of the degradation mechanism and identification of key factors determining the degradation kinetics are relatively lacking. In this presentation, we will introduce a number of our previous works for unveiling degradation pathways of Pt electrocatalysts, enabled with an advanced analytical platform, an online inductively coupled plasma mass spectroscopy (ICP-MS) coupled with an electrochemical flow cell (EFC). Effects of nature of reactants, electrochemical double-layer structure, time-scale, and various physicochemical parameters on their degradation have been thoroughly investigated. Based on these findings, we will discuss the possible interrelation of such parameters with catalytic stability.

Symposium : **MAT3-5**

Advanced Characterization in Materials Chemistry

Room 107 FRI 15:50

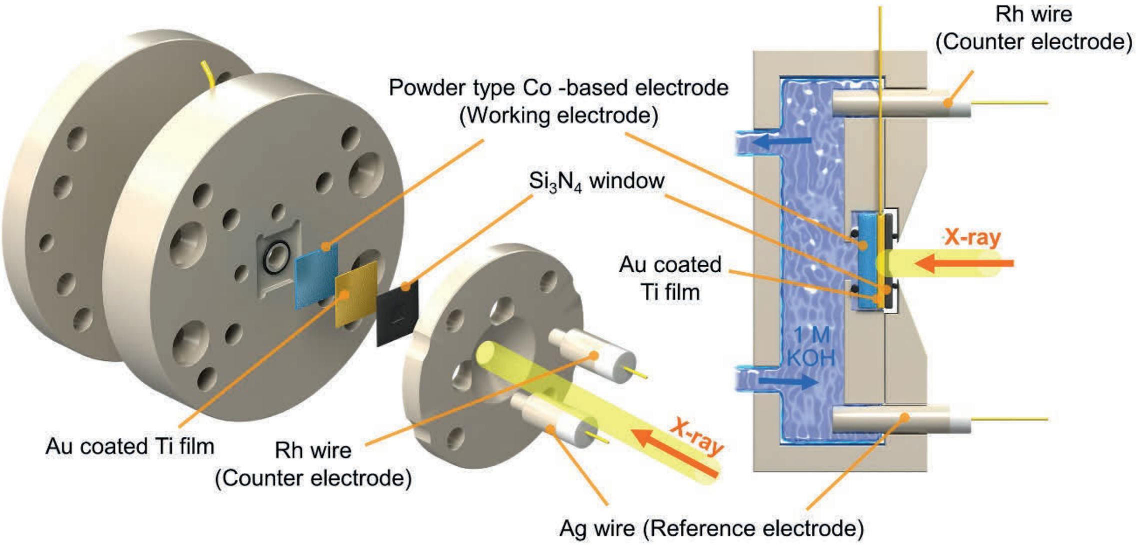
Chair: Byung Hyo Kim (Soongsil University)

Studies of electrocatalysts for water and CO_2 electrolysis via X-ray absorption spectroscopy (XAS)

Hyung-Suk Oh

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

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


Rh wire
(Counter electrode)
Powder type Co -based electrode
(Working electrode)
Si_3N_4 window
X-ray
Au coated
Ti film
1 M
KOH
Au coated Ti film
Rh wire
(Counter electrode)
X-ray
Ag wire (Reference electrode)

Symposium : **MAT3-6**
Advanced Characterization in Materials Chemistry
Room 107 FRI 16:10
Chair: Byung Hyo Kim (Soongsil University)

Design of stable electrocatalysts for CO2 reduction reaction

Yun Jeong Hwang

Chemistry Department, Seoul National University, Korea

Electrochemical CO2 conversion to valuable products has been recently highlighted and made significant progress in terms of current density as well as product selectivity. For instance, CO or formate can be achieved more than 95 % of Faradaic efficiency from electrochemical CO2 reduction reaction (CO2RR). Recent progress on the catalyst design have demonstrated over 70% of selectivity for C2 chemicals such as ethylene and ethanol. The next technical challenges in the catalyst development is achieving long-term stability for the target product. The factors that cause degradation of the CO2RR can be multiple. Hydrogen evolution reaction (HER) is one of the most competitive side reactions, and Faradaic efficiency for H2 increase as CO2RR performance is degradeded. Identicl location transimisison electron microscope (IL-TEM) shows that Ag nanoparticles can be dissolved and redeposited by CO2RR and the severe morphology changes had high correlation with the HER increase and thus decrease in CO production. Not only the morphological changes, but also metal impurities (ions) in the electrolyte can be detrimental for CO2RR because transition metal impurities can be reduced and deposited on the active sites of the Ag surface. We found Fe deactivate the CO production activity the most, and nitrogen doped carbon materials can exhibit high durability due to the low adsorption energy of Fe ions. Our studies suggest that carbon based modified catalysts can be stable electrocatalyst for CO2RR due to the high resistance of morphological changes and adhesion of the impurity metals. The activity can be further improved by introducing metal center single atom catalysts because it can adjust the binding energies of the adsorbate and contribute to selective production from CO2RR.

Award Lecture in Division : **ELEC1-4**
Electrochemistry for Post-Li Energy Storages
Room 108 THU 17:05
Chair: Jinho Chang (Hanyang University)

Evolution of Sensitization-based Photovoltaic Cells for Diverse Applications with Electrochemistry

Jae-Joon Lee

Research Center for Photoenergy Harvesting & Conversion Technology (phct), Dongguk University, Korea

The recent development and the research directions of the sensitization-based photovoltaic cells (DSPV) will be presented.

Since the first emergence of the dye-sensitized solar cells, lots of efforts have been paid for the commercialization of them while the highest attainable efficiency was still limited by far lower than that of the recently reported perovskite type solar cells. Recently, lots of further efforts were paid to enhance the transparency of dye-sensitized solar cells (DSSCs) with various color schemes so that they can be applied to the indoor-type photoenergy conversion/recycling system under very low light intensity condition as well as the conventional BIPV type applications. The current efforts are mostly focused on the diversification of dyes for various colors, development of the highly transparent electrode materials for both photoanode and counter electrode, designing of the highly stable and transparent semi-liquid electrolytes. The recent achievements were designed to make the large area module size up to 100 cm2 with the overall transmittance of 30% and efficiencies of 6, 5, 4 %, for red, green, and blue colored, respectively. These progresses expanded the application of DSPV to various areas including the development of DSPV-based artificial light cells (ALCs) for harvesting indoor-type low-intensity illumination for many self-powered IoT devices in conjunction with the development of the novel IoT-integrated smart lighting system for complete wireless interconnection as well as charging themselves. Similarly, DSPV system can be extended to develop a self-powered electrochemical biosensors for many smart wearable health care system. Another very challenging extension of this photovoltaic system is dye-sensitized photoelectrochemical energy conversion (DSPEC), which is designed to obtain some value-added fuels and chemicals very effectively and eco-friendly by electrochemical and photoelectrochemical degradation of many waste materials with a large molecular weight such as lignin and different types of micro plastics.

Symposium : **ELEC1-1**

Electrochemistry for Post-Li Energy Storages

Room 108 THU 15:40

Chair: Jinho Chang (Hanyang University)

Electrochemical behavior of iodide as redox active species in the positive electrode of zinc-polyiodide flow battery

Jung Hoon Yang

Korea Institute of Energy Research, Korea

The use of iodide as the positive redox-active species in redox flow batteries has been highly anticipated owing to its attractive features of high solubility, excellent reversibility, and low cost. However, the electro-oxidation reaction of iodide (I^-) is very complicated, giving various possible products such as iodine, polyiodides, and polyiodines. In particular, the electro-oxidation of I^-/I_3^- and I_3^-/I_2 occurs in competition depending on the applied potential. Although the former reaction is adopted as the main reaction in most redox flow batteries because I_3^- is highly soluble in an aqueous electrolyte, the latter reaction inevitably occurs together and a thick I_2-film forms on the electrode, impeding the electro-oxidation of I^-. In this study, we investigate the variation of the interface between the electrode and the electrolyte during the development of an I_2-film and the corresponding change in the charge-transfer resistance (R_{ct}).

Symposium : **ELEC1-2**
Electrochemistry for Post-Li Energy Storages
Room 108 THU 16:05
Chair: Jinho Chang (Hanyang University)

Towards Anti-Corrosion of Zinc Metal for Advanced Zinc-Air Batteries

Hyun Deog Yoo[*], **Sangram Keshari Mohanty**[1]

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

Researches on zinc metal-based (e.g., Zn-air) batteries have attracted considerable attention as a candidate for post lithium-ion batteries. Zinc is one of few metal anodes that are compatible in aqueous as well as non-aqueous electrolytes, providing a large theoretical capacity of 820 mAh g^{-1}. Zinc metal has been actively utilized as the anode for various primary batteries such as alkaline batteries, and it is under development for the advanced rechargeability. However, in aqueous electrolytes, zinc metal anode suffers from hydrogen evolution reaction (HER), by which zinc is irreversibly consumed or corroded continually. Therefore, anti-corrosion of zinc metal electrode has been a challenge in the development of Zn-based rechargeable batteries. Herein, we developed a chronocoulometric "deposition-rest-dissolution" method to quantify the corrosion rate without such interference from the deposition of Zn. The “deposition-rest-dissolution” method and electrochemical impedance spectroscopy confirmed that saturated $ZnSO_4$ (ca. 3.2 M) + 0.075 M Li_2SO_4 delivers the lowest corrosion rate compared to the other electrolytes probably due to the potential-dependent passivation in the sulfate-based electrolytes. The potential-dependent generation and decomposition of the passivation films were analyzed by electrochemical quartz crystal micro-balance (EQCM) technique. These approaches point to the importance of passivation phenomena for the stabilization of zinc metal electrodes, providing a practical strategy to enhance the (electro-)chemical stability. References 1.K. Y. Kwon et al., ACS Appl. Mater. Interfaces 12(38), 42612 (2020). 2.K. Y. Kwon et al., under review. 3.S. K. Mohanty et al., J. Phys. Chem. Lett. 12(24), 5748 (2021).

Symposium : **ELEC1-3**
Electrochemistry for Post-Li Energy Storages
Room 108 THU 16:30
Chair: Jinho Chang (Hanyang University)

Designer redox-active organic molecules for redox-enhanced electrochemical capacitors

Seung Joon Yoo

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

Fossil-based electricity generation causes global environmental problems. Renewable energy resources such as solar or wind have the potential to provide a clean and sustainable energy future, but the intermittent nature of these resources causes a mismatch of peak energy production and electricity demands. Thus, the rapid development of advanced electrochemical energy storage technologies is critical to stabilizing sustainable energy systems and the continuous delivery of their generated electricity.One approach in energy research is to utilize redox-active electrolytes that add faradaic charge storage to increase energy density of conventional supercapacitors. Aqueous redox-active electrolytes are simple to prepare and to up-scale; and, can be synergistically optimized to fully utilize the dynamic charge/discharge and storage properties of porous carbon based electrode systems. However, aqueous redox-enhanced electrochemical capacitors (redox ECs) have performed relatively poorly, primarily due to the cross-diffusion of soluble redox couples, reduced cycle life, and low operating voltages. In this presentation, we show how these challenges can be met by addressing the following topics including: (1) how important is surface adsorption to enhance effective concentration of redox ECs and thus energy density? (2) What properties of the organic molecules (viz., size, solubility, functional group) ensure increased effective concentration? (3) Can we define the roles of the pore sizes of the carbon electrode in promoting the charge storage of the redox species and correlate structure-property relationships with redox-active organic molecules? Simultaneously, investigation on the degree of cross-diffusion vs the ability of the charging product to be retained in the pores of the electrode will be discussed.

Symposium : **ELEC2-1**

Applications of Electrocatalysis for Renewable Energy Conversion

Room 108 FRI 09:00

Chair: Sung Yul Lim (Kyung Hee University)

Effect of Electric Field to Perovskite Quantum Dots for their Material/photophysical Properties

ChaeHyun Lee, Kyoungsoo Kim[1], YeJi Shin, Donghoon Han[1,*], Seog Joon Yoon[2,*]

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

All-inorganic lead-halide perovskite quantum dots (PQDs) (CsPbX3, where X is Cl, Br, or I) have been used successfully in optoelectronic applications, such as solar cells, light-emitting diodes, photocatalysts, and lasers. These PQDs work under electrochemical bias and/or illumination with charge separation/collection by interacting with the charge-transport medium. In this presentation, it will be discussed that the spectroelectrochemical characteristics of PQDs to understand the oxidation and reduction processes that occur during photoinduced charge transport or charge injection under electrochemical conditions. We also found that the PQDs underwent irreversible transformation to the precursor state of plumbate complexes under electrochemical conditions. Furthermore, in-situ spectroelectrochemical analysis demonstrated that hole-mediated electrochemical oxidation of PQDs resulted in their irreversible transformation. Finally, the results presented herein contribute to our understanding of the charge-transfer-mediated process in PQDs and enhance their application potential in optoelectronic devices.

Symposium : **ELEC2-2**
Applications of Electrocatalysis for Renewable Energy Conversion
Room 108 FRI 09:30
Chair: Sung Yul Lim (Kyung Hee University)

A RADICAL POLAR CROSSOVER STRATEGY IN ORGANIC ELECTROSYNTHESIS

Hyunwoo Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

In this session, two topics will be discussed in terms of a radical polar crossover strategy in organic electrosynthesis. First, an electrochemically driven strategy for the stereoselective synthesis of protected syn-1,2-diols from vinylarenes with N,N-dimethylformamide (DMF) will be presented. The newly developed system obviates the need for transition metal catalysts or external oxidizing agents, thus providing an operationally simple and efficient route to an array of protected syn-1,2-diols in a single step. This reaction proceeds via an electrooxidation of olefin, followed by a nucleophilic attack of DMF. Subsequent oxidation and nucleophilic capture of the generated carbocation with a trifluoroacetate ion is proposed, which gives rise predominantly to a syn-diastereoselectivity upon the second nucleophilic attack of DMF. Second, a radical hydrodifluoromethylation of alkenes via an electroreductively triggered two-pronged approach will be discussed. Despite their importance in pharmaceutical applications, synthetic routes to difluoromethylated pharmacophores are still very limited. To this end, we have devised a two-pronged strategy that enables hydrodifluoromethylation of a wide range of alkenes by means of reductive radical-polar crossover or direct hydrogen atom transfer from electroreductively generated carbon-centered radical intermediates. The newly developed strategy is generally valid to a wide range of alkenes and grant access to a late-stage modification of pharmacophores.

Symposium : **ELEC2-3**

Applications of Electrocatalysis for Renewable Energy Conversion

Room 108 FRI 10:00

Chair: Sung Yul Lim (Kyung Hee University)

Manipulating dynamic surface transformation of electrocatalysts for superior water oxidation

Jongwoo Lim

Division of Chemistry, Seoul National University, Korea

Rationally manipulating the in-situ formed catalytically-active surface of catalysts remains a tremendous challenge for highly-efficient water electrolysis. Here we present a cationic redox-tuning method to redirect dynamic surface restructuring from the same parent structure, for electrochemical oxygen evolution reaction (OER). Partially replacing oxygen of the layered transition metal oxides with halide modified redox transitions during the OER, which was monitored by operando X-ray absorption spectroscopy. Surface-restructured transition metal oxides showed an OER activity approximately two orders of magnitude higher than that of benchmark RuO2 and sustained this high activity for 500 h without degradation, making it among the best OER electrocatalysts ever reported. This work makes a stride in modulating surface restructuring and opens up new opportunities to design superior OER electrocatalysts via tuning cationic redox.

Symposium : **ELEC2-4**
Applications of Electrocatalysis for Renewable Energy Conversion
Room 108 FRI 10:30
Chair: Sung Yul Lim (Kyung Hee University)

3D printing with functional inks for 3D Printed Electronics

Seung Kwon Seol

Smart 3D Printing Research Team, Korea Electrotechnology Research Institute, Korea

Three-dimensional (3D) printing, also known as additive manufacturing, is widely regarded as a revolution in manufacturing technology, with significant promise for electronic applications; this field is known as 3D printed structural electronics. However, it is difficult to obtain functional 3D structures for electronics, although we can easily produce plastic or metallic 3D objects with coarse resolution via various commercial 3D printing methods, such as stereolithography (SLA), fused deposition modeling (FDM), or selective laser sintering (SLS). Finding the appropriate printing approach for the achievement of functional 3D structures with high spatial resolution remains one of the major challenges in the field of 3D printed electronics. Here, we demonstrate a novel strategy for multiple-materials 3D printing at room temperature in ambient air conditions. The 3D micro- and nanoarchitectures are printed by an omnidirectional accurate control of a micrnozzle filled with functional inks. A simple modulation of the ink leads to 3D printing for multiple-materials, such as graphene, carbon nanotube (CNT), metal oxide, metal, magnet, and their composite. Successful demonstrations of 3D printed functional components are also described herein. We believe that this approach paves the way for efficient multi-material 3D printing with high spatial resolution, which will ultimately lead to important advancements in 3D printed electronics.

Symposium : **EDU-1**
Development of Textbooks on Chemistry Education for Pre-service Teachers
Room 109 THU 15:40
Chair: Seounghey Paik (Korea National University of Education)

Developing a textbook on teaching chemistry

Jeonghee Nam

Department of Chemical Education, Pusan National University, Korea

This book was written in response to the demands of educators who teach chemistry method courses in the pre-service chemistry teacher training course. This book focuses on developing and updating prospective and practicing chemistry teachers' pedagogical content knowledge. The 5 chapters of the book discuss the most essential theories from science education and each of the chapters apply the theory to examples from the chemistry classroom. The chapters provide the nature of chemistry, science and chemistry curriculum, the practice of secondary level of chemistry textbook analysis, teaching method based on teaching and learning theory, and assessment. In this presentation we will discuss what is our intention and how this book help chemistry educators in the field.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Symposium : **EDU-2**
Development of Textbooks on Chemistry Education for Pre-service Teachers
Room 109 THU 16:05
Chair: Seounghey Paik (Korea National University of Education)

Science Teaching Models for Chemistry Instruction

HyunJu Park, Hyunjung Kim[1,*]

Faculty of Chemistry Education, Chosun University, Korea
[1]*Department of Chemistry Education, Kongju National University, Korea*

The purpose of this study was to summarize and organize the science teaching models for constructing a textbook of 'Practicum in Chemistry Teaching Materials' that implement pre-service teachers' chemistry instructions. Eight science teaching models were selected by analyzing textbooks related to science education theory, textbook research and guidance, and science teaching model, which were textbooks published in the field of science education in Korea and used in pre-service teacher education. The selection criteria for the teaching model were as follows. First, it was covered in the science teaching model of the 'Secondary Teachers Recruitment Examination' for chemistry teacher. Second, it was included in the major textbooks in the field of science education used in pre-service teacher education. Third, it included science teaching models that published the results of the study on the effectiveness or usefulness of the science teaching model in the study of science education. The eight science teaching models were as follows: Inquiry model, discovery model, model of learning cycle, model of conceptual change, generative learning model, STEAM, STS, and POE. There were several issues in writing this chapter. Despite the same science teaching model, there have been cases in which the instructional steps differ or the terms used differ depending on the textbook. It was necessary to discuss whether all science teaching models used in modern science education should be included in the textbook. Although a chemistry instruction activity of science teaching model was an example, it could be understood by students as a typical example, which would act limitedly on the development of students' teaching abilities. We hope that this textbook will help chemistry prospective teachers and teachers professional development of the Pedagogical Content Knowledge.

Symposium : **EDU-3**
Development of Textbooks on Chemistry Education for Pre-service Teachers
Room 109 THU 16:40
Chair: Seounghey Paik (Korea National University of Education)

Characteristics of Foreign Chemistry Curriculum

Hyunjung Kim

Department of Chemistry Education, Kongju National University, Korea

The purpose of this study was to compose the 'Chemistry textbook research and instruction' to improve preservice teachers' expertise in chemistry teaching by comparing the characteristics of the chemistry curriculum in major countries that can give implications to the Korean chemistry curriculum. In the foreign chemistry curriculum, we looked at the curriculum in the United States, Estonia, and Singapore. The United States has traditionally been a major benchmark country when designing Korea's national curriculum, while Singapore and Estonia reflect international educational trends such as 'OECD Education 2030' in their curriculum, and also top performers in achievements in PISA and TIMSS. The United States looked at National Science Education Standards and Next Generation Science Standards. The contents of the science curriculum are divided into three dimensions, , and eight Science Practices are presented by clarifying and expanding the concept of scientific exploration. The Estonian curriculum is based on achievement standards such as for each grade group, and then and achievement standards are presented. The Singapore curriculum is centered on the spirit of scientific inquiry, and the practice of inquiry is based on . The achievement standards are presented in conjunction with three aspects of knowledge, skills, and attitudes and using behavioral verbs for each of the four to five topics covered by each grade cluster.

Symposium : **EDU-4**
Development of Textbooks on Chemistry Education for Pre-service Teachers
Room 109 THU 17:05
Chair: Seounghey Paik (Korea National University of Education)

Introduction to the “Chemistry Textbook Analysis” section of “Research and Teaching Method for Chemistry Textbooks”

Seounghey Paik

Department of Chemical Education, Korea National University of Education, Korea

Many chemistry education researchers present various examples of analyzing chemistry sections in middle and high school science textbooks and high school chemistry textbooks. Representative examples include analysis cases according to educational goals, representation, models, and inquiry activities. By presenting these research cases in the “Chemistry Textbook Analysis” section of “Research and Teaching Method for Chemistry Textbooks” taught by pre-service chemistry teachers, the content of the textbook was structured so that chemistry teachers could analyze chemistry-related textbooks and develop their own optimal educational materials.

Symposium : **ENVR-1**
Advances in Electrochemistry Using Ion Exchange Membranes for Environmental and Energy Applications
Room 110 THU 15:40
Chair: Jin-Soo Park (Sangmyung University)

Recent Progress in Development of High-Performance Cation-Exchange and Anion-Exchange Membranes for Electrochemical Energy Conversion System

Byungchan Bae

Fuel Cell Laboratory, Korea Institute of Energy Research, Korea

Electrochemical energy conversion system including fuel cells and electrolyzer has been highlighted as a future energy technology because it did not follow Carnot cycle and exhaust carbon dioxide. The cost competitiveness and life cycle are the most challenging for the successful initiation of the renewable energy market. The polymer electrolyte membrane has been one of the essential components that can influence the performance and durability of electrochemical energy conversion systems. Although a perfluorinated electrolyte membrane has been widely used as a cation exchange membrane, it suffered from high price and durability. This seminar will present recent research results and trends that can solve the shortcomings of existing perfluorinated electrolyte membranes. In addition, research trends and developments of anion exchange electrolyte membranes for alkaline membrane fuel cells and electrolyzers, which are being actively researched in recent years, will also be presented.

Symposium : **ENVR-2**
Advances in Electrochemistry Using Ion Exchange Membranes for Environmental and Energy Applications
Room 110 THU 16:10
Chair: Jin-Soo Park (Sangmyung University)

Importance of Ion Exchange Membrane in Capacitive Deionization.

Hanjoo Kim

PUREECHEM Co., Ltd., Korea

Due to the recent continuous environmental pollution and water shortage, research on desalination technology is being actively conducted. Capacitive deionization (CDI) technology based on electrochemistry has a high recovery rate and low energy consumption, so interest among desalination technologies is increasing. This technology is a technology that adsorbs ions by electrostatic force by applying an electric potential in a low range where no chemical reaction occurs based on the principle of an electric double layer. This technology is controllable with a high recovery rate, energy-efficient, and environmentally friendly technology, which significantly compensates for the shortcomings of other desalination technologies. While CDI technology has excellent potential, commercialization is difficult due to the lack of application examples of the technology.The early CDI technology consisted only of an electrode that adsorbs or desorbs ions and a spacer of a flow path, but recently, it has been developed and applied by combining an ion exchange membrane, and its performance is about 40% superior to that of CDI without an ion exchange membrane. However, the cost of the ion exchange membrane is quite expensive, more than 50% of the material cost of CDI technology. Among the most popular desalination technologies, it is difficult to enter the market because the initial facility cost is higher than that of the RO technology. However, CDI technology with excellent durability has excellent economical maintenance cost. Therefore, it is urgent to develop an ion exchange membrane that is economical and suitable for CDI technology. As a result, the market for electrochemical water treatment technology is expected to expand compared to competing technologies.

Symposium : **ENVR-3**

Advances in Electrochemistry Using Ion Exchange Membranes for Environmental and Energy Applications

Room 110 THU 16:40

Chair: Jin-Soo Park (Sangmyung University)

Understanding the phenomenon of capacity decay through Nafion membranes in vanadium redox flow battery

Jung Hoon Yang

Korea Institute of Energy Research, Korea

Capacity decay in vanadium redox flow batteries during charge–discharge cycling has become an important issue because it lowers the practical energy density of the battery. The battery capacity tends to drop rapidly within the first tens of cycles and then drops more gradually over subsequent cycles during long-term operation. This study analyzes and discusses the reasons for this early capacity decay. The imbalanced crossover rate of vanadium species was found to remain high until the total difference in vanadium concentration between the positive and negative electrolytes reached almost 1 mol/L. To minimize the initial crossover imbalance, we introduced an asymmetric volume ratio between the positive and negative electrolytes during cell operation. Changing this ratio significantly reduced the capacity fading rate of the battery during the early cycles and improved its capacity retention at steady state.

Symposium : **ENVR-4**

Advances in Electrochemistry Using Ion Exchange Membranes for Environmental and Energy Applications

Room 110 THU 17:10

Chair: Jin-Soo Park (Sangmyung University)

Principle and application of bipolar electrodialysis

Jeon soo Hong, TAKEO KAWAHARA[1,*]

Research Institute, CHANGJOTECHNO CO., Korea
[1]ASTOM Corporation, Japan

The bipolar membrane electrodialysis (BMED) is the technology for the conversion of a salt into its corresponding acid and base. The bipolar membranes carry out the splitting of water into protons and hydroxide ions in electrodialysis water splitting. Bipolar membranes are a special type of layered ion exchange membrane where the two ion exchangeable polymer layers where one is only permeable for the anions and another only for cations. In combination of electrodialysis for salt separation, BMED could be applied in various industry areas due to excellent long-term stability, high permselectivity, good mechanical stability, etc. In this study, the various processes for the production of acids and bases from NaCl, Na2SO4 and KF solutions were introduced.

Oral Presentation : **POLY.O-1**
Oral Presentation for Young Polymer Scientists
Room 101 THU 09:00
Chair: Min Sang Kwon (Seoul National University)

Phase-separated Hydrogels with Embedded Nanogels to Improve Shrinking and Re-swelling Processes

Taehun Chung, Jihoon Han, Younsoo Kim*

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

Thermoresponsive hydrogels have been attracting attention in a variety of functional materials, because they exhibit a volume phase transition phenomenon near physiological temperatures. However, the slow kinetics and small volume shrinkage of bulk poly(*N*-isopropylacrylamide) (PNIPAAm) hydrogels upon heating greatly limit their practical application. Here, we propose a novel type of thermoresponsive hydrogels that show improved shrinking and re-swelling. By using globular structure of PNIPAAm in salt solution, it is possible to synthesize phase-separated hydrogels with ultrafast and large shrinkage than normal type of hydrogels. Furthermore, we incorporated simply synthesized nanogels in phase-separated hydrogels. As a result, hydrophilic and ionic nanogels effectively improved the kinetics of re-swelling. In this presentation, synthetic strategy of thermoresponsive hydrogels and improved kinetics of them will be discussed.

Oral Presentation : **POLY.O-2**
Oral Presentation for Young Polymer Scientists
Room 101 THU 09:10
Chair: Min Sang Kwon (Seoul National University)

Single Chain Folding of Sequence-Controlled Graft Copolymers into Subdomain-Defined Polymer Nanoparticles

Jiyun Nam, Jae suk Lee[1], YongJoo Kim[2], Myungeun Seo[3,*]

chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Advanced Materials Engineering, Gwangju Institute of Science and Technology, Korea*
[2]*School of Advanced Materials Engineering, Kookmin University, Korea*
[3]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

We developed a methodology for the precision synthesis of core cross-linked star (CCS) polymers inspired by protein folding. Well-defined graft copolymers were synthesized with a designated number of side chains and dimerizable groups by graft-through ring opening metathesis polymerization. Intrachain photodimerization converges the backbone into a compact globular conformation, translating the molecular information written on the 1D chain into the 3D globular nanoparticle. Unprecedented control over structural parameters of CCS polymer was achieved. Folding of sequence-controlled graft copolymers containing different side chains allowed us to spatially control formation of distinct subdomains in the CCS polymers, as evidenced by drastically different self-assembly behavior.

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

Oral Presentation for Young Polymer Scientists

Room 101 THU 09:20

Chair: Min Sang Kwon (Seoul National University)

A High Toughening effect of Highly Branched Polycaprolactone-grafted Cellulose Copolymer on a fully Bio-based PLA Blend Material

Roshaan Zafar

Materials Science and Engineering, Seoul National University, Korea

Due to the pending issue regarding the generation and disposal of petroleum based plastics, the use of bio-based plastics has been of great interest in the scientific and industrial fields. Among various biopolymers, polylactic acid (PLA), an aliphatic polyester typically derived from bio-resources such as plant starches, is one of the most essential bio-polymer candidate for various industrial applications. However, the applications of PLA are significantly limited when compared to the petrochemical-based materials owing to its inherent characteristics such as brittleness. In this study, a fully bio-based PLA blend with highly branched polycaprolactone-grafted cellulose (Cghbp) was prepared and characterized to enhance the toughness of PLA. The Cghbp was synthesized by ring-opening copolymerization (ROCP) method and its chemical structure was analyzed by 1H-NMR, 13C-NMR and FT-IR. The PLA bio-blends, i.e., PLA-Cghbp series were fabricated with precisely controlled amount of Cghbp by solvent casting. The prepared PLA-Cghbp bio-blends were found by FT-IR to be physically intact. The WXRD and DSC analyses indicated that the addition of Cghbp disrupted the ordered chain structures of PLA resulting in the changes in PLA crystalline phase. It was evident that as the amount of Cghbp increased, the glass transition temperature (Tg) of PLA-Cghbp blends gradually decreased. When 5wt% of Cghbp amount was adjusted, the tensile toughness of PLA-Cghbp was 56.1MJ/m3, which is 3 times higher than the toughness of neat PLA. This significant increase in tensile toughness may be attributed to the fact that when an optimal amount of Cghbp is added to PLA, the synergistic effect of cellulose and its highly branched side chains are capable of inducing flexibility to the rigid PLA chains.

Oral Presentation : **POLY.O-4**
Oral Presentation for Young Polymer Scientists
Room 101 THU 09:30
Chair: Min Sang Kwon (Seoul National University)

Antimicrobial PEGtides: A Modular Poly(Ethylene Glycol)-Based Peptidomimetic Approach to Combat Bacteria

Minseong Kim, **Byeong-Su Kim**[1,*]

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

Despite their high potency, the widespread implementation of natural antimicrobial peptides is still challenging due to their low scalability and high hemolytic activities. Herein, we address these issues by employing a modular approach to mimic the key amino acid residues present in antimicrobial peptides, such as lysine, leucine, and serine, but on the highly biocompatible poly(ethylene glycol) (PEG) backbone. A series of these PEG-based peptides (PEGtides) were developed using functional epoxide monomers, corresponding to each key amino acid, with several possessing highly potent bactericidal activities and controlled selectivities, with respect to their hemolytic behavior. The critical role of the composition and the structure of the PEGtides in their selectivities was further supported by coarse-grained molecular dynamic simulations. This modular approach is anticipated to shed a light on the design principles necessary for the future development of antimicrobial polymers.

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

Oral Presentation for Young Polymer Scientists

Room 101 THU 09:40

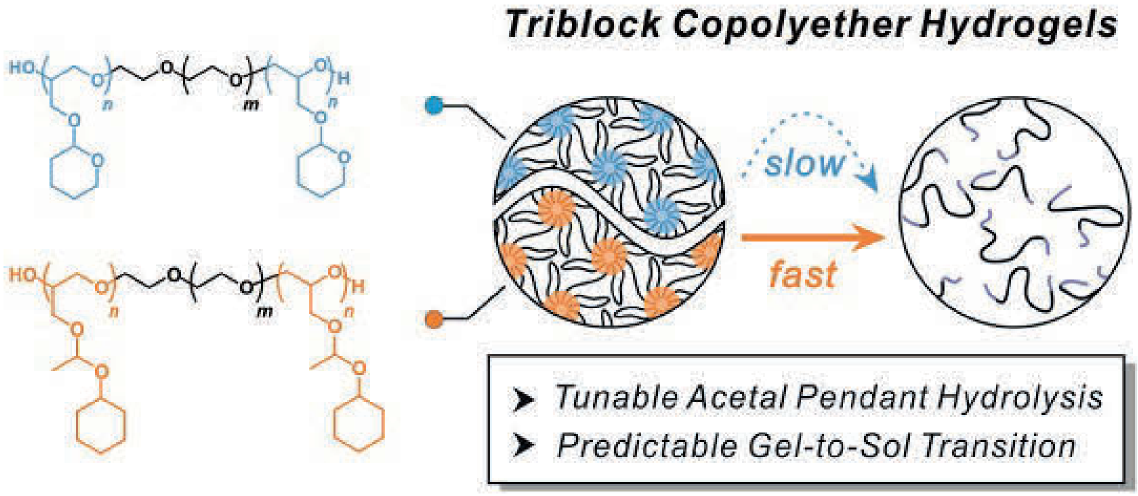
Chair: Min Sang Kwon (Seoul National University)

Hydrolysis-Driven Viscoelastic Transition in Triblock Copolyether Hydrogels with Acetal Pendants

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

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

While the hydrolytic cleavage of ester groups is widely exploited in degradable hydrogels, the scission at the midst of chain backbones can bring dramatic changes in the mechanical properties of the hydrogels. However, the predictive design of the mechanical profile of the hydrogels is a complex task, mainly due to the randomness of the location of chain scission. To overcome this challenge, we herein present degradable ABA triblock poly(ethylene oxide)-based hydrogels containing an A-block bearing acetal pendant, which provides systematically tunable mechano-temporal properties of the hydrogels. In particular, hydrophobic endocyclic tetrahydropyranyl or exocyclic 1-(cyclohexyloxy)ethyl acetal pendants are gradually cleaved by acidic hydrolysis, leading to the gel-to-sol transition at room temperature. Most importantly, a series of dynamic mechanical analyses coupled with ex situ NMR spectroscopy revealed that the hydrolysis rate can be orthogonally and precisely tuned by changing the chemical structure and hydrophobicity of acetal pendants. This study provides a new platform for the development of versatile degradable hydrogels in a highly controllable manner.


Triblock Copolyether Hydrogels
HO
O
n
m
H
slow
fast
Tunable Acetal Pendant Hydrolysis
Predictable Gel-to-Sol Transition

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

Oral Presentation for Young Polymer Scientists

Room 101 THU 09:50

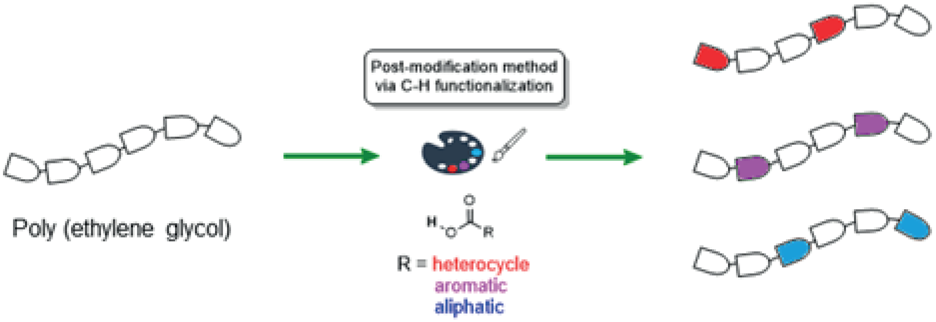
Chair: Min Sang Kwon (Seoul National University)

Synthesis of Poly[(Ethylene Glycol)-co-(Acyloxylated Ethylene Glycol)] via Post-modification of Poly(Ethylene Glycol)

Se Jong Kim, Jeung Gon Kim*

Department of Chemistry, Jeonbuk National University, Korea

As known, Poly Ethylene Glycol(PEG) is hydrophilic polymer, commonly used in batteries, medicine, pharmacy, and various industry. To improve its performance, the synthesis of functionalized PEG has been of interest. Usually, functionalized-PEG is synthesized from epoxide monomers. However, the scopes of monomers is limited due to functional group incompatibility and uneven reactivity. To overcome these limitations, the synthesis of functionalized-PEG via post-modification polymerization is pursued. In this study, using the C-H functionalization strategy, PEG was directly functionalized using several kinds of functional group to obtain the corresponding functionalized-PEG without decreasing in molecular weight. Furthermore, we tried to introduce bioactive substances into PEG. The current status of our research will be presented in this symposium.



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

Oral Presentation for Young Polymer Scientists

Room 101 THU 10:00

Chair: Min Sang Kwon (Seoul National University)

Design of novel water-soluble purely organic photocatalyst for aqueous PET-RAFT polymerization

Yungyeong Lee, **Min Sang Kwon**[*]

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

We report a design of a novel water-soluble purely organic photocatalyst (PC) and its application to aqueous photoinduced electron/energy transfer reversible addition fragmentation chain transfer (PET-RAFT) polymerization. Ultra-low concentrations of the designed PC (5 ppm to monomers) enabled an oxygen-tolerant (or oxygen-accelerated) PET-RAFT polymerization of a variety of acrylate and acryl amide monomers in water and buffer. In addition, using chain transfer agent-modified bovine serum albumin, protein-polymer conjugates were successfully synthesized via grafting-from method under mild reaction conditions (e.g., room temperature and visible-light irradiation) – notably in the absence of deoxygenation process or any additives such as sacrificial agents. We anticipate this novel PC to be applied to a variety of organic and polymerization reactions in aqueous and/or biologically relevant media; for example, to afford an expanded library of protein-polymer conjugates with diverse functionalities.

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

Oral Presentation for Young Polymer Scientists

Room 101 THU 10:10

Chair: Min Sang Kwon (Seoul National University)

Supramolecularly Associated Block Copolymer Networks Forming Adhesive Ionogels for On-Skin type Strain Sensor

Sol An, Myungwoong Kim*

Department of Chemistry, Inha University, Korea

The development of flexible, wearable, and portable sensors has drawn attentions rapidly in recent years. However, durability of the wearable electronic devices has been limited due to the weak adhesiveness on skin not allowing dynamic motions during strenuous exercise. Here, we demonstrate that introducing dual-component micellar systems comprising intra- and inter-micellar hydrogen bonding block copolymers in an ionic liquid, which are applicable to the stretchable, and self-adhesive on-skin-type strain sensor for motion monitoring. We have successfully synthesized diblock copolymers of poly(t-butyl styrene-b-(2-vinyl pyridine-r-methyl acrylate) and poly(t-butyl styrene-b-(4-(2-tetrahydropyranyloxy)styrene-r-methyl acrylate) via reversible addition-fragmentation chain-transfer polymerization where 4-(2-tetrahydropyranyloxy)styrene units produced phenolic-OH groups by acidolysis. The polymeric micelle clusters organized by self-assembly in ionic liquid were associated via hydrogen bonding between pyridine and phenol. The designed ionogels exhibited high stretchability, toughness, and thermal stability as well as self-adhesion properties owing to the achieved supramolecular structure and the strong hydrogen bonding. These results highlight that effective physical adhesion in dry state through the complex interactions between the ionogel and skin surface, improving accurate detection of dynamic movements.

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

Oral Presentation for Young Polymer Scientists

Room 101 THU 10:20

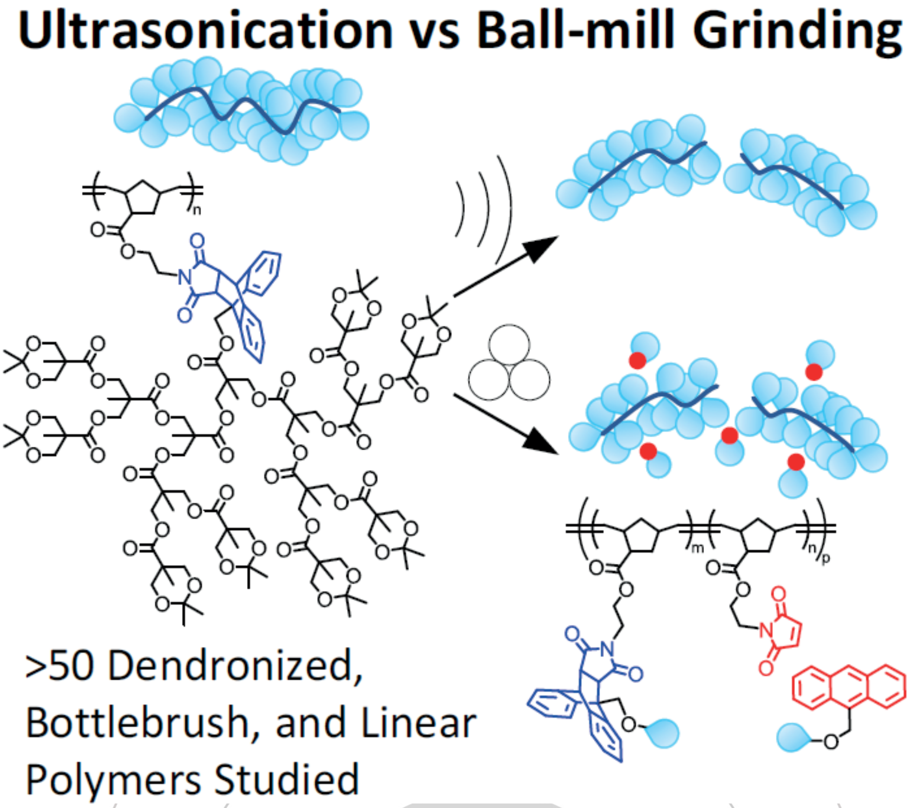
Chair: Min Sang Kwon (Seoul National University)

Solution- and Solid-state Mechanochemical Reactivity of Bottlebrush Polymers and Dendronized Polymers

Jinkyung Noh, Gregory Peterson[1,*], Tae-Lim Choi[*]

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

Besides the degree of polymerization (DPs) or lengths of the polymer backbones, their side chains could also affect their mechanochemical reactivity under external stimuli. Recently, we explored the degradation kinetics of linear, bottlebrush, and dendronized polymers in solution-state (ultrasonication) and solid-state (ball-mill grinding) systematically. Broad polymer scope with identical backbone structures (of varying DPs) and diverse kinds and sizes of side chains revealed the critical parameters that influence polymers' chain scission events. Furthermore, by using graft multi-mechanophore polymers where the mechanophores are located at the backbone-(bulky) arm junction in every repeating unit, we could figure out the key factors to obtain high mechanophore activation efficiency. These results are expected to be important background information for designing mechano-responsive polymer systems.


Ultrasonication vs Ball-mill Grinding
>50 Dendronized,
Bottlebrush, and Linear
Polymers Studied
n
m
n
p

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

Oral Presentation for Young Polymer Scientists

Room 101 THU 10:30

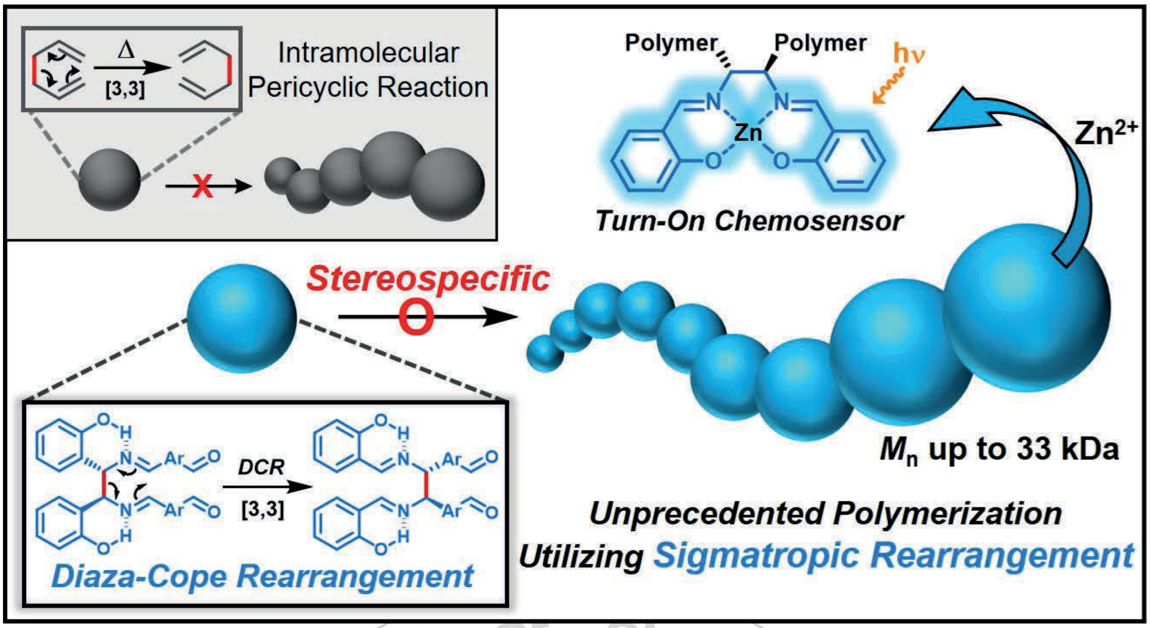
Chair: Min Sang Kwon (Seoul National University)

Tandem Diaza-Cope Rearrangement Polymerization: Turning Stereospecific Intramolecular Reaction into Powerful Polymerization to Give Enantiopure Zn^{2+} Sensor

Soon-Hyeok Hwang, Tae-Lim Choi*

Division of Chemistry, Seoul National University, Korea

[3,3]-Sigmatropic rearrangement is a powerful and reliable pericyclic reaction, allowing for the stereoselective construction of C–C bond. However, this rearrangement cannot be applied to polymerization other than the post-modification of side-chains because it is an intramolecular reaction, which intrinsically forms and breaks the bond simultaneously. Herein, we report a new tandem diaza-Cope rearrangement polymerization (DCRP) to synthesize high-molecular-weight polymers up to 33.3 kDa with excellent stability against hydrolysis due to resonance-assisted hydrogen bond (RAHB). A mechanistic investigation by *in situ* ^{1}H NMR experiments suggests that this polymerization proceeds by a rapid DCR process, forming an enantiospecific C–C bond that occurs almost simultaneously with imine formation. This polymerization produces also chiral polymers containing enantiopure salen moieties, which lead to high-performance Zn^{2+}-selective turn-on chemosensors with up to 73-fold amplification. We also investigated that their optical activities and sensing performances are heavily dependent on the reaction temperature, which significantly affects the stereoselectivity of DCR.


Δ
[3,3]
Intramolecular
Pericyclic Reaction
Polymer
Polymer
hν
Zn
Zn²⁺
Turn-On Chemosensor
Stereospecific
DCR
[3,3]
Ar
Diaza-Cope Rearrangement
Mn up to 33 kDa
Unprecedented Polymerization
Utilizing Sigmatropic Rearrangement

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

Oral Presentation for Young Polymer Scientists

Room 101 THU 10:40

Chair: Min Sang Kwon (Seoul National University)

Molecular-Orientation-dependent Ion Transport Dynamics in Organic Mixed Ionic Electronic Conductors

Ji Hwan Kim, Myung-Han Yoon[*]

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

Despite the importance of transient behavior in organic mixed conductors, few studies have been conducted on the optical, electrochemical, and structural characteristics of materials that influence ion drift and the associated transient responses of corresponding organic electrochemical transistors (OECTs). In this study, we show that the molecular orientation of a mixed conducting polymer system with glycol side chains can be independently controlled by changing the co-monomer unit (2,2'-bithiophene or phenylene) used with a novel 1,4-dithienylphenylene-based monomer with a high glycol side-chain density. Two polymers with similar mixed conductivity and electrochemical properties except for molecular orientation were successfully synthesized. The transient/frequency response measurement of the OECT suggested that the molecular orientation affects the length of the ion-drift pathway, which is directly correlated with ion mobility, resulting in different transient responses in OECT devices. Our study provides general insights into the molecular-orientation-dependent ion migration properties of polymeric mixed conductors and the material/device design principles governing their applications in biomolecular sensing, biosignal recording, neuromorphic devices, and other fields.

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

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 09:45

Chair: Jungwon Park (Seoul National University)

Memories of the Late Professor Si-Joong Kim and My Academic Journey at POSTECH

Joon Won Park

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

POSTECH and Division of Inorganic Chemistry in KCS are my grateful platform to enjoy the journey during the last 31 years. The late Professor Si-Joong Kim had been a great mentor and guardian of all of us. We are quite lucky to have him, and literally all KCS members are beneficiary of him. I remember that he attended meetings of our Division until recently, and gave precious advice with a full of love. It is my great honor to receive this Award named after him. Let's keep his spirit and love alive continuously.After doctoral study at Caltech and postdoctoral training at Northwestern University, I started my independent academic career at POSTECH in 1990. During the first ten years, we touched three different topics, organometalllic catalysts for polymerization, catalytic hydrolysis of phosphate esters, and wet surface chemistry. The last subject is most productive for me, and in 2000 I came up with a new idea to immobilize biomolecules on solid substrates in a rational way (later the approach is named NanoCone technology), and improved performance for microarrays and biochips was the expected outcome. With generous support of POSCO, I was able to push the project forward. Luckily, I had a chance to introduce the approach to a UK biophysicist, and was proposed to use such surface coating for bio-AFM (Atomic Force Microscopy). My story to medical diagnostics began with such a fortunate encounter. Actually, it took almost 17 years to arrive at use of such approach for liquid biopsy, one of my dreams sprung at late 40s. Commercialization of the approach for human-kind is now a new dream.

Award Lecture in Division : **INOR.O-9**
Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)
Room 203 THU 10:15
Chair: Jungwon Park (Seoul National University)

From DGIST-1 to DGIST-7

Yesub Keum, Byeongchan Lee, Seonghun Park, Bongkyeom Kim, Jinhee Park[*]

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

Our research group aims to develop porous functional materials, mainly metal-organic frameworks (MOFs) and metal-organic polyhedral (MOPs). In the MOFs and MOPs, metal clusters as the joints are interconnected to multitopic organic ligands as linkers in the network structures. Thus, their physicochemical properties are highly tailorable through the judicious combinations of the building blocks. Further, the crystalline nature of the MOFs facilitates in-depth study of the structure- property relationships. We have been tried to harness these advantages of the MOFs and MOPs for their applications in gas sorption, ion exchanges, catalysis, and sensing. The newly synthesized MOFs and MOPs in our group have been named as DGIST-X (X=1, 2, 3…). This presentation will cover the structures and properties of DGIST-1 to DGIST-7. In addition, post-synthetic modification (PSM), especially covalent PSM, which expands the versatility of functional groups and thus promotes porosities and stabilities of the MOFs and MOPs will be discussed.

Award Lecture in Division : **INOR.O-10**

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 10:45

Chair: Jungwon Park (Seoul National University)

Metal-Organic Frameworks: Structure and Their Applications in Storage, Separation and Transport

Minyoung Yoon

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

Metal-Organic Frameworks (MOFs) have developed after a pioneering contribution by Prof. Robson in the early 1990s. Due to the permanent porosity, the MOFs were considered the analog of zeolite, which was applied to the same application areas of zeolites. In addition, the reticular chemistry based on the coordination theory and the diversity of organic ligands allows drastic expansion of the candidate MOF materials. Although MOFs were mainly used in gas sorption (storage) and catalysis, the application field was expanded to separation, magnetism, fluorescence, and transport, which are directly related to the chemical nature and the framework structure. In our group, we mainly focus on the structural nature of MOFs and their property related to the structure. Recently, we prepared a series of 2D-porous network, $Zn_2(AIP)_2(pillar)$ (AIP: 5-aminoisophthalic acid, pillar: 4,4'-bipyridyl and its analogs) that shows breathing property responding to the organic solvent molecules. By utilizing the breathing nature, the frameworks were used for selective adsorption of C_8 alkyl aromatic isomers (such as xylenes). The frameworks showed different selectivity depending on the framework as well as C_8 isomers. For the practical application of the material, breakthrough experiments for C_8 isomer mixture separation were demonstrated. Furthermore, the porous network provides a unique platform for the transport of ions such as a proton. The metal formates ($M(HCO_2)_2$, M = Mg, Co, and Ni) were employed for the study of proton conduction in MOFs. Interestingly, the framework shows unique structural transformation depending on the relative humidity, which was confirmed by powder X-ray diffraction analysis. Although the crystal structure transformation was non-reversible, the hydrated metal formates show unusual and reversible crystal-amorphous transformation depending on the relative humidity, which controls proton conduction on/off switching. The details of this work will be presented.

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

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 09:00

Chair: Jungwon Park (Seoul National University)

Hexapodal Tricationic Amphiphiles for Anion-Induced and Aggregation-Enhanced Light Emission

Soohyung Kim, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Molecular recognition in water is an unperfected art in synthetic supramolecular chemistry. Especially, the recognition of anions in water remains a key challenge. While prevailing paradigms utilize rigid cavities for ion recognition, selective detection of large, non-spherical, and charge-diffuse anions is more challenging if one relies solely on electrostatic interactions. We show that multipodal polycationic receptors function as anion-responsive light-emitters in water. A combination of ion-pairing and aggregation event produce selective fluorescence “turn on” response, as demonstrated by perchlorate as a non-spherical hydrophobic anion model. Detailed structural analysis by X-ray crystallographic and NMR spectroscopic studies revealed that a synergetic interplay of C–H···anion hydrogen bonding and tight anion–π^+ contacts are responsible for this supramolecular phenomenon. By systematically varying the alkyl pendant chain length or introducing pH-responsive functional groups, we also demonstrated that the response profile and threshold of this signaling event can be controlled at the molecular level to differentiate various hydrophobic anions based on the size and hydrophobicity. In this presentation will be discussed key design principles, synthetic implementations, and rational strategies to achieve high-sensitivity detection of soft non-spherical anions in water.

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

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 09:06

Chair: Jungwon Park (Seoul National University)

Regulation of the Nitrile Activation of a Peroxocobalt(III) Complex using Redox-Inactive Metal Ions

Kyungmin Kim, Jaeheung Cho[1,*]

Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Chemistry, UNIST, Korea*

Redox-inactive metal ions play vital roles in biological O_2 activation and oxidation reactions of various substrates. Recently, we showed a distinct reactivity of a peroxocobalt(III) complex bearing a tetradentate macrocyclic ligand, $[Co^{III}(TBDAP)(O_2)]^+$ (**1**) (TBDAP = *N,N'* -di-*tert*-butyl-2,11-diaza[3.3](2,6)pyridinophane), toward nitriles that afforded a series of hydroximatocobalt(III) complexes, $[Co^{III}(TBDAP)(R\text{-}C(=NO)O)]^{2+}$ (R = Me (**3**), Et and Ph). In this study, we report the effects of redox-inactive metal ions on nitrile activation of **1**. In the presence of redox-inactive metal ions such as Zn^{2+}, La^{3+}, Lu^{3+}, and Y^{3+}, the reaction does not form the hydroximatocobalt(III) complex, but instead gives peroxyimidatocobalt(III) complexes, $[Co^{III}(TBDAP)(RC(=NH)O_2)]^{2+}$ (R = Me (**2**) and Ph (**2^{Ph}**)). These new intermediates were characterized by various physicochemical methods including X-ray diffraction analysis. The rates of the formation of **2** are found to correlate with the Lewis acidity of the additive metal ions. Moreover, complex **2** was readily converted to **3** by the addition of a base. In the presence of Al^{3+}, Sc^{3+}, or H^+, **1** is converted to $[Co^{III}(TBDAP)(O_2H)(MeCN)]^{2+}$ (**4**) and further reaction with nitriles did not occur. These results reveal that the reactivity of the peroxocobalt(III) complex **1** in nitrile activation can be regulated by the redox-inactive metal ions and their Lewis acidity. DFT calculations show that the redox-inactive metal ions stabilize the peroxo character of end-on Co–η^1-O_2 intermediate through the charge reorganization from a Co^{II}-superoxo to a Co^{III}-peroxo intermediate. A complete mechanistic model explaining the role of the Lewis acid is presented.

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

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 09:12

Chair: Jungwon Park (Seoul National University)

Minimalistic Principles for Designing Small Molecules with Multiple Reactivities against Pathological Factors in Dementia

Mingeun Kim, Mi Hee Lim*

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

Multiple pathogenic elements, including reactive oxygen species, amyloidogenic proteins, and metal ions, are associated with the development of neurodegenerative disorders. In this presentation, we report minimalistic redox-based principles for preparing compact aromatic compounds by derivatizing the phenylene moiety with various functional groups. These molecular agents display enhanced reactivities against multiple targets such as free radicals, metal-free amyloid-β (Aβ), and metal-bound Aβ that are implicated in the most common form of dementia, Alzheimer's disease (AD). Mechanistic studies reveal that the redox properties of these reagents are essential for their function. Specifically, they engage in oxidative reactions with metal-free and metal-bound Aβ, leading to chemical modifications of the Aβ peptides to form covalent adducts that alter the aggregation of Aβ. Moreover, the administration of the most promising candidate significantly attenuates the amyloid pathology in the brains of AD transgenic mice and improves their cognitive defects. Our studies demonstrate an efficient and effective redox-based strategy for incorporating multiple functions into simple molecular reagents.[1]Reference1.M. Kim, J. Kang, M. Lee, J. Han, G. Nam, E. Tak, M. S. Kim, H. J. Lee, E. Nam, J. Park,S. J. Oh, J.-Y. Lee, J.-Y. Lee, M.-H. Baik, M. H. Lim, *J. Am. Chem. Soc.* **2020**, *142*, 8183-8193.

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

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 09:18

Chair: Jungwon Park (Seoul National University)

Ultramicroporous Metal-Organic Frameworks with Selective Adsorption of Ethane over Ethylene

Minjung Kang, Jong Hyeak Choe, Hyojin Kim, Daewon Kim, Hyein Park, Chang Seop Hong[*]

Department of Chemistry, Korea University, Korea

Ethylene, a high-value chemical for industrial polymer production, is mostly produced through the steam cracking process of fossil fuels. Additional purification is required to obtain polymer-grade ethylene (>99.95%) due to ethane impurities of 5%-10%. For practical applications, potential adsorbents must exhibit high structural stability while maintaining high ethane adsorption even at low pressures. We synthesized ultramicroporous MOFs and evaluated its ethane and ethylene adsorption performance. The MOFs exhibit selective uptake of ethane over ethylene and enhanced structural stability under humid condition. The selectivity was calculated by the IAST and dynamic gas separation experiments were also performed on ethane/ethylene mixtures. Detailed synthetic scheme and specific properties will be given in the presentation.

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

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 09:24

Chair: Jungwon Park (Seoul National University)

A Golgi Apparatus-targeting Fluorescent Probe for the Selective Sensing of Formaldehyde

Jinheung Kim*, Fortibui Maxine Mambo[1]

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

Formaldehyde (FA) is in the production of numerous household chemical goods. Here, a fluorescent chemosensor for FA is designed and prepared using a selective organ-targeting probe containing naphthalimide as a fluorophore and hydrazine as a FA-binding site. The amine group of the hydrazine reacts with FA to form a double bond and this condensation reaction is accompanied by a shift in the absorption band of the probe from 438 nm to 443 nm upon the addition of FA. Further, the addition of FA is shown to enhance the emission band at 532 nm relative to the very weak fluorescent emission of the probe itself. Moreover, a high specificity is demonstrated toward FA over other competing analytes such as calcium ion, magnesium ion, acetaldehyde, benzaldehyde, salicylaldehyde, glucose, glutathione, sodium sulfide, sodium hydrosulfide (NaHS), hydrogen peroxide, and the tert-butylhydroperoxide radical. A typical two-photon dye incorporated into the probe provides intense fluorescence upon excitation at 800 nm, thus demonstrating the potential application as a two-photon fluorescent probe for FA sensing. Furthermore, the probe is shown to exhibit a fast response time for the sensing of FA at room temperature and to facilitate intense fluorescence imaging of breast cancer cells upon exposure to FA, thus demonstrating its potential application for the monitoring of FA in living cells. Moreover, the presence of the phenylsulfonamide group allows the probe visualize dynamic changes in the targeted Golgi apparatus. Hence, the as-designed probe is expected to open up new possibilities for unique interactions with organ-specific biological molecules with potential application in early cancer cell diagnosis.

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

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 09:30

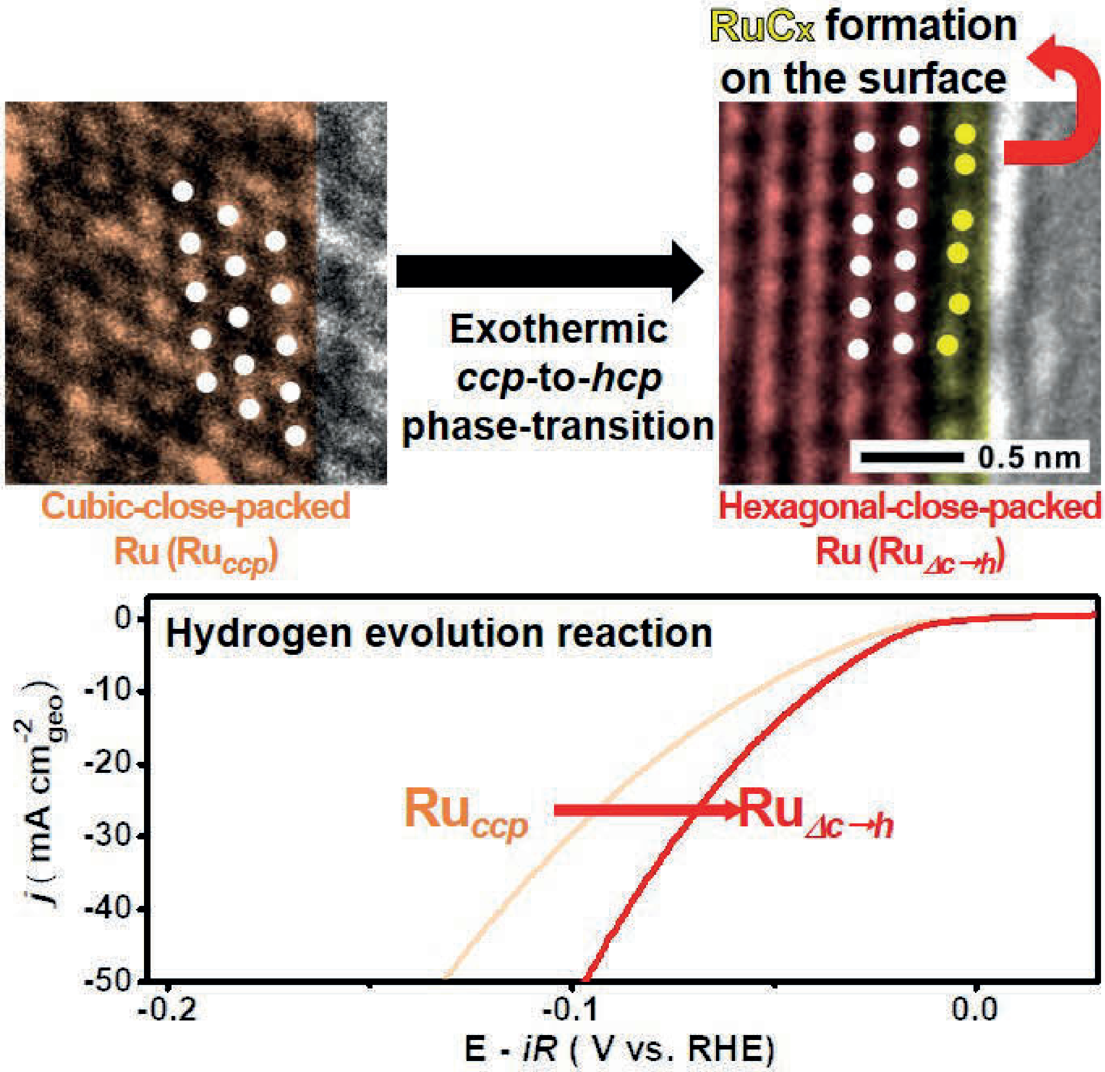
Chair: Jungwon Park (Seoul National University)

Crystal Phase Transition creates RuC_X Nanosurface towards the Hydrogen Evolution Reaction in Alkaline Media

Jeonghyeon Kim, Hee Jin Kim, Sang-Il Choi*

Department of Chemistry, Kyungpook National University, Korea

Although meta-stable crystal structures have received much attention owing to their utilization in various fields, their phase-transition to a thermodynamic structure has attracted comparably little interest. In the case of nanoscale Ru crystals, such an exothermic form cubic-close-packed Ru (Ru_{ccp}) to hexagonal-close packed Ru (Ru_{hcp}) phase-transition releases high energy within a confined surface area and reconstructs surface atomic arrangement in a short time. Thus, this high-energy nanosurface may create novel crystal structures when some elements are supplied. In this work, we discovered the Ru_{ccp}(111) plane changes to the Ru_{hcp}(002) plane during the phase-transition by allowing atom slippage in the close-packing system with in-situ high-resolution transmission electron microscopy (HRTEM) and high-temperature X-ray diffraction. Then, after the exothermic phase-transition, a novel ruthenium carbide (RuC_X, $X < 1$) phase was created on the surface of the Ru nanocrystal, as determined by HRTEM and high-resolution photoemission spectroscopy analyses. When, the electrocatalytic hydrogen evolution reaction was tested in alkaline media, the RuC_X exhibited a much lower overpotential and good stability relative to the counterpart Ru-based catalysts and the state-of-the-art Pt/C catalyst. The density functional theory calculations predicted that the local heterogeneity of the outermost RuC_X surface promotes the bifunctional HER mechanism by providing catalytic sites for both H adsorption and facile water dissociation.


RuCx formation on the surface
Exothermic ccp-to-hcp phase-transition
0.5 nm
Cubic-close-packed Ru (Ru$_{ccp}$)
Hexagonal-close-packed Ru (Ru$_{\Delta c \rightarrow h}$)
Hydrogen evolution reaction
Ru$_{ccp}$
Ru$_{\Delta c \rightarrow h}$
j (mA cm$^{-2}_{geo}$)
0
-10
-20
-30
-40
-50
-0.2
-0.1
0.0
E - iR (V vs. RHE)

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

Oral Presentation of Young Scholars in Inorganic Chemistry (inc. Award Lectures)

Room 203 THU 09:36

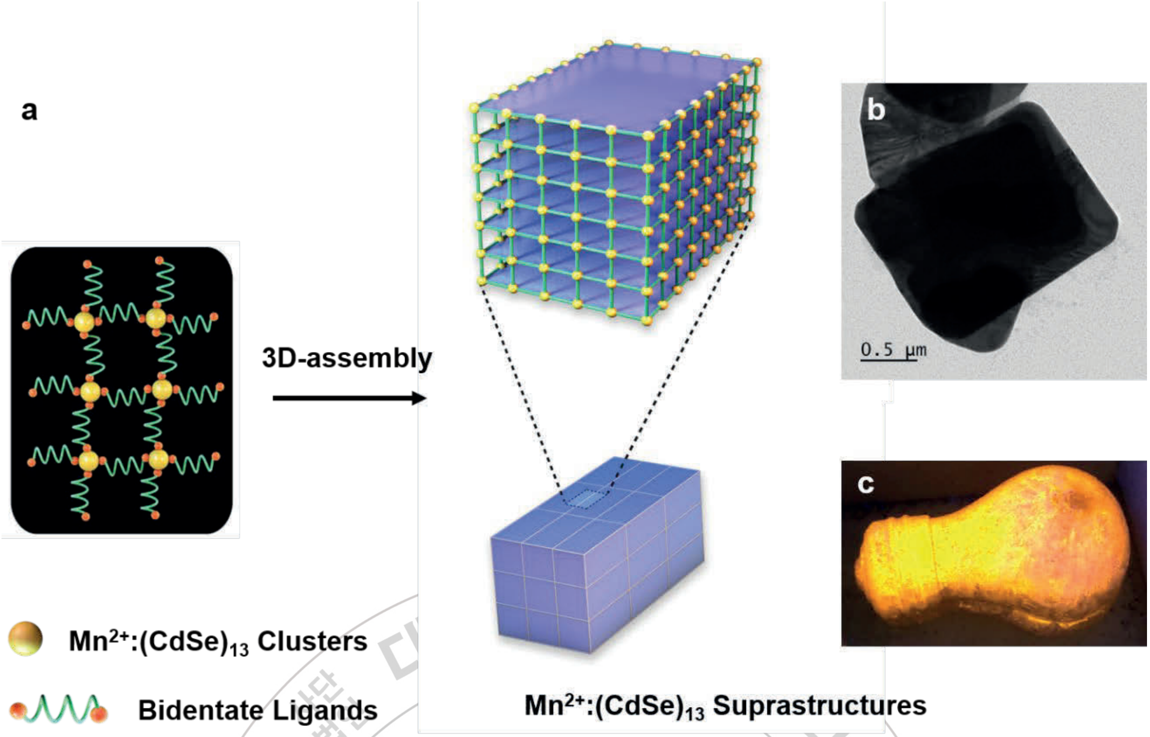
Chair: Jungwon Park (Seoul National University)

Highly Luminescent and Catalytically Active Magic Semiconductor Clusters-Based Metal−Organic Frameworks

Woonhyuk Baek, Taeghwan Hyeon*

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

Semiconductor magic-sized nanoclusters (MSCs) composed of exact number of metal chalcogenide unit have exhibited intriguing optoelectronic and physicochemical properties which cannot be attained in ensemble nanocrystals(NCs) counterparts. However, ambient instability has hindered their extensive utilization exploiting their single size.Controlled bottom-up assembly of nano-building blocks is one of the primary aims of nanotechnology with high stability and tunable structure, consequently, utilized in potential applications in sensing, catalysis, and other fields. However, the size and structure of conventional NCs inevitably are in distribution resulting in ensemble properties in assembly, which impede deep understanding single collective properties in nano-assembly.Herein, we explored the periodic assembly of MSCs nanoscale building blocks through organic linkers to overcome such limitations and further foster their properties. We designed a diamine-ligated self-assembly heat-up process to assemble Mn2+:(CdSe)13 and Mn2+:(ZnSe)13 MSCs into three- and two-dimensional superstructures (SSs), respectively, achieving enhanced stability and solid-state photoluminescence quantum yields (from


a
3D-assembly
Mn^{2+}:$(CdSe)_{13}$ Clusters
Bidentate Ligands
Mn^{2+}:$(CdSe)_{13}$ Suprastructures
b
0.5 μm
c

Oral Presentation : **PHYS.O-1**
Oral Presentations for Young Physical Chemists
Room 103 THU 09:00
Chair: Myung Won Lee (Pukyong National University)

Uncertainty Estimation for AI-Accelerated Materials Design

Juhwan Noh, Yousung Jung*

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

Design of new materials has been recognized as an essential element in various applications, but it still largely depends on experts' intuition or try-and-error approach. In this regard, computational high throughput screening (HTS) has emerged as a practical approach for acceleration of the discovery of new materials with target properties in recent years. However, the major bottleneck in HTS is a large computational cost of density functional theory (DFT) calculations to obtain target properties, limiting the size of explorable chemical space. Thus, recent machine learning (ML) framework have been proposed to overcome this challenge by leveraging structure-property relations from the materials database, [1] but there still exist two major challenges in the current ML framework: (1) requiring DFT-relaxed structures to make reliable predictions and (2) model-dependent uncertainty-included screening performance. In this talk, therefore, I will present the Bayesian ML frameworks to handle the latter two challenges. [2,3] Our benchmark against an our previous all DFT-HTS task [4] demonstrates significant decrease in the required DFT calculations by a factor of >50 compared to the previous approach. [2] Also, I will present the improved uncertainty estimation approach for model-independent HTS performance by utilizing the error-embedding of the latent space. [3]

[1] J. Noh et al. *Chem. Sci.* 2020, **11**, 4871-4881.
[2] J. Noh et al. *J. Chem. Inf. Model.* 2020, **60**, 1996-2003.
[3] J. Noh et al. *submitted.*
[4] J. Noh et al. *Chem. Commun.* 2019, **55**, 13418-13421.

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

Oral Presentations for Young Physical Chemists

Room 103 THU 09:15

Chair: Myung Won Lee (Pukyong National University)

Why Additional Corrections Terms Compensate DFA?

Suhwan Song, Eunji Sim[*]

Department of Chemistry, Yonsei University, Korea

The most popular way to handle exchange-correlation (XC) energy as a functional of an electron density is to use Kohn-Sham ansatz. From localized density approximation (LDA) to double-hybrid (DH) functionals, there has been a various approximated version of XC potential, but almost all XC potentials based on Slater exchange term is lack of describing non-covalent interaction energies due to its exponentially decaying feature instead of Coulombic 1/r decaying. The underestimation of the weakly bonded interactions is therefore compensated from the additional dispersion correction term such as Grimme's disp2, 3, and 4 or Vydrov's VV10. Almost all additional correction term assist standard XC approximated functional to remedy the underestimation of the energy by fitting their inherent parameters to those non-covalent interactions such as pi-pi interaction, intra-molecular interactions, hydrogen-bonding, and halogen bonding. Here, we explain why such an additional correction term performs well even with the fitting process as a density error point of view. Also, we discuss how to improve the performance of the reaction where additional dispersion correction terms worsen the result.

Oral Presentation : **PHYS.O-3**
Oral Presentations for Young Physical Chemists
Room 103 THU 09:30
Chair: Myung Won Lee (Pukyong National University)

Localized Excitons in 2D Magnetic Semiconductor $CrPS_4$

Suhyeon Kim, Sunmin Ryu*

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

Ultrathin chromium thiophosphate ($CrPS_4$) with near IR photoluminescence (PL) emission is a reference system of 2D antiferromagnetic semiconductors.[1] In this study, we revealed the remarkable exciton landscape of $CrPS_4$ by observing temperature-dependent PL signals using micro-PL spectroscopy and time-correlated single-photon counting (TCSPC). At 4 K, the phosphorescence band including its vibrational peaks was shown. In contrast, the fluorescence band was exhibited at room temperature, attributed to the activated back intersystem crossing from the excited doublet state (^2E_g) to the excited quartet state ($^4T_{2g}$) at higher temperatures. These optical transitions can be understood based on the crystal field theory used to explain the electronic structure of molecular systems. In addition, it has a heavier effective mass of electrons than transition metal dichalcogenides (TMDs).[2] The exciton of $CrPS_4$ can be more localized than that of recent 2D semiconductors such as TMDs. In the results of time-resolved PL (TRPL) measurements, few-layer systems exhibited biphasic decay kinetics attributed to the two different surrounding environments for Cr^{3+} ions acting as the exciton recombination center. The dependence of PL lifetime on sample thickness was related to the defects-assisted non-radiative decay. Reference[1] J. Lee, T. Ko, J. Kim, H. Bark, B. Kang, S. Jung, T. Park, Z. Lee, S. Ryu, and C. Lee, ”Structural and Optical Properties of Single- and Few-Layer Magnetic Semiconductor $CrPS_4$”, ACS Nano, 2017, 11, 10935-10944.[2] H. Zhuang, J. Zhou, “Density Functional Theory Study of Bulk and Single-layer Magnetic Semiconductor $CrPS_4$”, Physical Review B, 2016, 94, 195307.

Oral Presentation : **PHYS.O-4**
Oral Presentations for Young Physical Chemists
Room 103 THU 09:45
Chair: Myung Won Lee (Pukyong National University)

Direct Observation of Distinct Amyloid Aggregation Dynamics in Water and Heavy Water Using Two-Dimensional Infrared (2D-IR) Spectroscopy

So Yeon Chun, MyungKook Son, Chae Ri Park, Chaiho Lim, Hugh I. Kim[*], Kyungwon Kwak[*], Minhaeng Cho[*]

Department of Chemistry, Korea University, Korea

Amyloid proteins that undergo self-assemblies to form insoluble fibrillar aggregates have attracted much attention due to their role in biological and pathological significance in amyloidosis. Various spectroscopic techniques, including infrared (IR) spectroscopy, have made efforts to track the appropriate structural dynamics indicative of complex mechanisms of the aggregation process. However, IR studies are limited in water (H2O) by the signal overlap of H-O-H bending mode of H2O and amide I band and are done in heavy water (D2O), which raises fundamental questions regarding the isotopic effect of D2O on protein dynamics. We aim to understand the different amyloid aggregation dynamics of insulin (INS) in H2O and D2O using two-dimensional IR spectroscopy (2D-IR). Utilizing the advantages of 2D-IR, we could directly monitor the structural changes during INS fibrillation in H2O as well as D2O. Comparison of 2D-IR results reveals that the unique quaternary structure of INS causes distinct fibrillation pathways of INS in H2O and D2O. Furthermore, with the aid of several biophysical analyzes and other spectroscopic techniques, we demonstrate further insight into the mechanical details of the distinct structural transition dynamics of INS in H2O and D2O. This study provides an innovative 2D-IR approach to study the protein dynamics in H2O instead of D2O.

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

Oral Presentations for Young Physical Chemists

Room 103 THU 10:00

Chair: Woon Yong Sohn (Chungbuk National University)

Reproducing Quasi-Crystalline and Amorphous Structures via Dendritic Oligomers: Mechanisms for Singlet Exciton Fission

Juno Kim, Dongho Kim[*]

Department of Chemistry, Yonsei University, Korea

Pentacene dendritic structures as a set of delicate model systems which mimic amorphous and quasi-crystalline phase of solid-states are introduced. As weakly interacting structures, phenylene-bridged TIPS-pentacene (Pc) dendrimers were prepared by controlling the number of chromophores and linking positions (trimer, tetramer, and hexamer). In addition, a tightly-packed hexamer whose substituents were changed to mesityl group of lesser steric hindrance was synthesized to reproduce quasi-crystalline structures of substantial pi-pi orbital overlaps. By reproducing amorphous and quasi-crystalline structures in solid-states, the role of through-bond/space interactions, CT intervention, and entropy enhancement by oligomerization in singlet exciton fission (SEF) process is comprehensively understood.From a molecular viewpoint, the oligomerization strategy created multiple channels for the generation of multiexcitonic triplet pairs via both through-bond and –space interactions. From the viewpoint of structural heterogeneity, the generation of multiexcitonic triplet pairs of different boundness and a SEF hot spot were proposed as coupling strengths are sensitive to the local structures. In addition, by virtue of the tight-packing structure, charge transfer-coupled multiexciton state was observed and entropic contribution was proposed during the generation of pure triplet pair configuration within the dendritic structure.

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

Oral Presentations for Young Physical Chemists

Room 103 THU 10:15

Chair: Woon Yong Sohn (Chungbuk National University)

Anisotropic circular dichroism spectroscopy of jet-cooled molecules

Changseop Jeong, Ji Yeon Yun[1], Jiyoung Heo[2], Nam Joon Kim[*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of chemistry, Chungbuk Natioanl University, Korea*
[2]*Department of Green Chemical Engineering, Sangmyung University, Korea*

Circular dichroism (CD) spectroscopy is one of the most powerful methods to investigate the structures and reactions of chiral molecules. The CD of molecules with fixed spatial distribution is called anisotropic CD (ACD). ACD spectroscopy has been extensively used to probe the orientation of macromolecules in anisotropic medium. Here, we have obtained the resonant two photon ionization CD (R2PICD) spectra of rotational P-, Q-, and R-branch transitions for the origin bands of conformers A, B, and C of (-)PED using a dual laser beam method. It is found that the CD values of the P-, Q-, and R-branch transitions of the origin bands are different from each other. Furthermore, the CD values of the rotational transitions of conformers A and C do not exhibit mirror images between (+) and (-)PED. These results are explained by ACD phenomena of jet-cooled molecules undergoing the P-, Q-, and R-branch transitions.

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

Oral Presentations for Young Physical Chemists

Room 103 THU 10:30

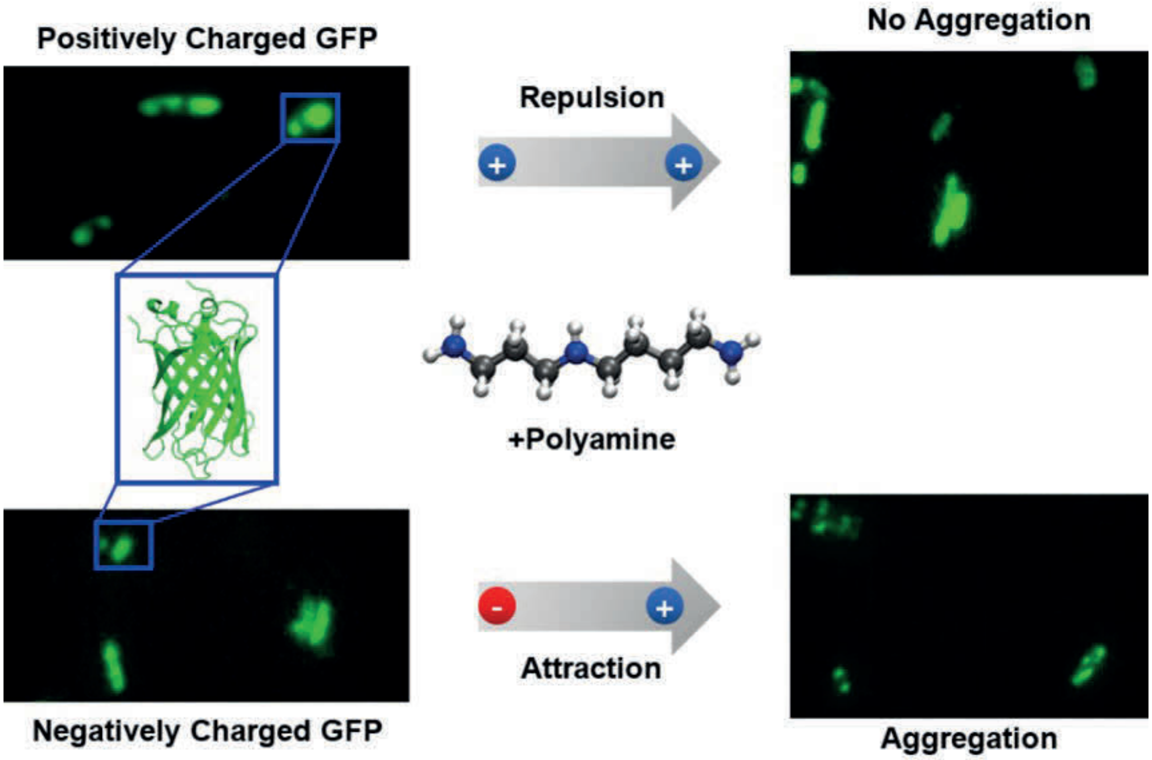
Chair: Woon Yong Sohn (Chungbuk National University)

Small Biomolecules Induce Protein Aggregation through Charge-Charge Interaction

Minchae Kang, **Sang Hak Lee**[1,*]

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

Protein aggregation, also referred to as phase separation, has been the subject of much research in biology, biophysics, and chemistry. Protein aggregation can function either to promote normal cellular metabolism or to disturb normal cellular functions. The chemical mechanism underlying protein aggregation is not clearly understood. It is well-known that many aggregated proteins are highly charged, either positively or negatively. Thus, we hypothesized that protein aggregation is mediated by small charged biomolecules: negatively charged nucleoside triphosphate (NTP) interacting with positively charged proteins and positively charged polyamine interacting with negatively charged proteins. In this study, we employed super-charged green fluorescence protein (scGFP) to study how charged proteins are aggregated through charge-charge interaction with small charged biomolecules in cells. Here, when expressing scGFP in E-coli, positively charged (+28) GFPs were found to aggregate with NTP and negatively charged (-27) GFPs aggregated with polyamine molecules. We thereby conclude that the small charged biomolecules are the main driver to induce protein aggregation in cells.


Positively Charged GFP
No Aggregation
Repulsion
+
+
+Polyamine
-
+
Attraction
Negatively Charged GFP
Aggregation

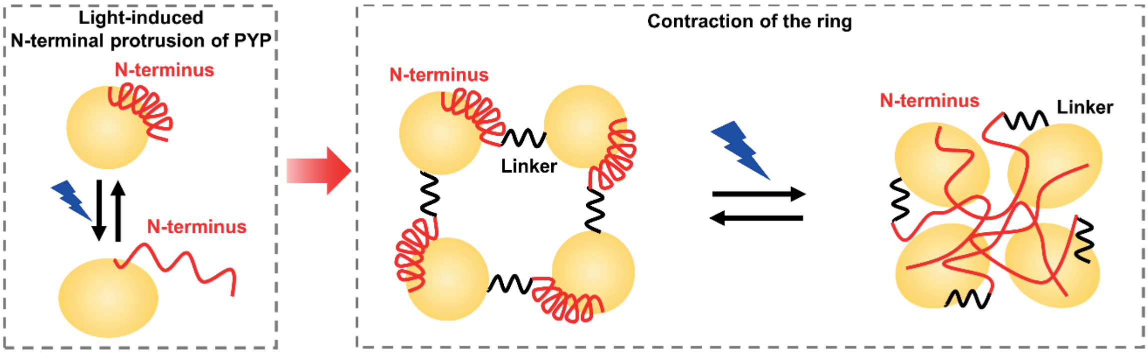
Oral Presentation : **PHYS.O-8**
Oral Presentations for Young Physical Chemists
Room 103 THU 10:45
Chair: Woon Yong Sohn (Chungbuk National University)

Reversible molecular switch based on circular photoactive protein oligomers exhibits unexpected light-induced contraction

Sang Jin Lee, Tae Wu Kim[1], Hyotcherl Ihee[*]

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

Molecular switches are molecules that can reversibly switch between two stable states in response to external stimuli such as light, temperature, voltage, pH, and ligands. Since molecular switches provide useful applications in various fields, numerous studies have been reported on molecular switches. Nevertheless, the practical applications of molecular switches are limited by the precise control and characterization of both structural properties and motion. In particular, the accurate and comprehensive structural characterization of molecular switching motion is a highly challenging task and has been rarely reported. Here, we generate a novel protein-based molecular switch composed of photoactive-protein building blocks and demonstrate its rapid and reversible conformational changes in response to irradiation. The structural and photochromic properties of photoactive yellow protein (PYP) were harnessed to construct circular oligomer PYPs (coPYPs) of desired sizes. Based on the light-induced N-terminal protrusion of monomer PYP, we expected the structure of coPYPs would expand upon irradiation. However time-resolved X-ray solution scattering (TRXSS) data reveal that the final photoproduct of a coPYP actually undergoes contraction instead of expansion. This work not only provides an approach to engineering a novel protein-based molecular switch based on circular oligomers of a well-known protein unit but also demonstrates the importance of actually characterizing the structural dynamics of designed molecular switches.


Light-induced
N-terminal protrusion of PYP
N-terminus
N-terminus
Contraction of the ring
N-terminus
Linker
N-terminus
Linker

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 09:00

Chair: Sung Yul Lim (Kyung Hee University)

Subnanoscale probing of nanojunction using heterogeneous gap-mode Raman spectroscopy†

Dongha Shin

department of chemistry, Inha University, Korea

Symmetric bifunctional molecule-linked nanogap structures have been frequently used in nanoelectronics, it is still challenging to discriminate the phenomenon that happened at both interfacial regions with subnanoscale resolution. Here, we fabricated platinum–silver or silver–platinum heterogeneous nanogap structures using a symmetric isocyanide terminated molecule, and using surface-enhanced Raman spectroscopy, we investigated the electrochemical potential-dependent change in the two distinguishable isocyanide stretching bands in such structures. Counterintuitively, we observed that the isocyanide group at the nanoparticle surface experiences more enhanced effective potential than the one at the plate surface, and this is attributed to the nanoparticle-induced effects rather than the potential drop that conventionally occurred due to molecular resistance. Our study provides a novel strategy allowing the subnanoscale investigation of numerous interfacial phenomena, which could not be achieved via conventional spectroscopic techniques.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 09:06

Chair: Sung Yul Lim (Kyung Hee University)

SERS-based serodiagnosis of acute febrile diseases using nanopopcorn microarray platforms

Kihyun Kim, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

It is essential to develop sensitive and accurate diagnosistic tool for acute febrile diseases because the current gold standard method called immunofluorescent assay (IFA) cannot give accurate and objective readout. To resolve this problem, we developed a surface-enhanced Raman scattering (SERS)-based immunoassay platform for the diagnosis of scrub typhus and murine typhus, which are the most common acute febrile diseases in South Korea. A microarray device, composed of multiple gold nanopopcorn substrates capable of detecting disease-specific biomarkers, was used as a multiplex SERS-based assay platform. We analyzed Raman signals from different titers of Orientia tsutsugamushi and Rickettsia typhi specific human IgG/IgM antibodies, which are biomarkers of two typhus diseases, and the peak intensity was plotted against each titer concentration range to generate calibration curves. The LODs of titer concentrations for O. tsutsugamushi IgG/IgM and R. typhi IgG/ IgM are determined to be 20.4, 7.03, 16.8 and 12.5, respectively. These LOD values all meet the cut-off values (256, 16, 128, and 64) used for clinical diagnosis, unlike conventional ELISA method. These results show that our SERS-based assay platform can accurately diagnose two typhus diseases with high sensitivity.

Oral Presentation : **ANAL1.O-3**
Oral Presentation of Young Analytical Chemists I
Room 104 THU 09:12
Chair: Sung Yul Lim (Kyung Hee University)

Analysis of the effects of NO gas in cancer cells based on NO-generating electrochemical system

Chae ri Park, Jeeyoung Ma[1], MyungKook Son, Dongjoon Im, Sooyeon Chae, Kyoungsuk Jin[2,*], Hugh I. Kim[*]

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

In vivo tissue activity control is achieved by delivering various physiological molecules between cells inside and outside the tissue. Therefore, when studying life phenomena and diseases at the molecular level, it is necessary to simultaneously analyze the interactions between biological molecules in cells and various organic and inorganic molecules and ions. However, a clear understanding is difficult due to the complexity of cell groups in the sample. Furthermore, studying the reactivity and adaptability of cells by external gas molecules is experimentally very limited. In this study, we applied an electrochemical system to control NO gas delivery to cells and investigated the effect of NO gas on cells by concentration. We placed A549 cells in a NO-generating electrochemical system and exposed these cells to NO gas. Distinct cell viability was observed based on the applied NO concentration. We also developed an available system to adjust the distance from cells to the NO-generating working electrode to control the degree of exposure to NO gas. Our results provide a materialized platform capable of observing the gas reactivity of cells by external gases to understand the cellular responses to gas molecules in the actual complex intracellular and extracellular microenvironments.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 09:18

Chair: Sung Yul Lim (Kyung Hee University)

Multifunctional Optical Probes in Dynamic Biological Environments Using Mesoporous Silica Shell Coated Single Gold Nanorods

Geun Wan Kim, Ji Won Ha[*]

Department of Chemistry, University of Ulsan, Korea

Mesoporous silica coated gold nanorods (AuNRs@mSiO_2) are promising multifunctional orientation probes that can be employed in biological studies due to their anisotropic optical properties, enhanced stability, and excellent biocompatibility. In this paper, we characterized the optical properties of single AuNRs@mSiO_2 under dark-field (DF) microscopy and differential interference contrast (DIC) microscopy and demonstrated the application as orientation probes in a dynamic biological environment. First, we obtained the periodic DIC images and intensities of single AuNRs@mSiO_2 at their localized surface plasmon resonance (LSPR) wavelengths with high sensitivity. Furthermore, we successfully tracked the real-time rotational motions of the AuNRs@mSiO_2 on the live cell membranes with millisecond temporal resolution. this study will be beneficial for potential applications, as a multifunctional optical probe that can determine the orientation of probe and delivery appropriate drug to target cell.

Oral Presentation : **ANAL1.O-5**
Oral Presentation of Young Analytical Chemists I
Room 104 THU 09:24
Chair: Sung Yul Lim (Kyung Hee University)

Pilot study for biomarker discovery of prostate cancer using proteomics

Miseon Jeong, Wonryeon Cho[*]

Department of Chemistry, Wonkwang University, Korea

Prostate-specific antigen (PSA) is a protein biomarker used in the early diagnosis of prostate cancer (PCa) in clinics. However, the PSA level is elevated not only in PCa but also in other prostate diseases, resulting in false-positive diagnoses. This pilot study aims to discover biomarkers that enable a more accurate early diagnosis of PCa by detecting PSA from prostate tissues in PCa patients and then identifying the proteoforms of PSA specific to PCa. However, there is difficulty in detecting PSAs present in trace amounts among abundant proteins present in tissues. First, the proteome was profiled by applying shotgun proteomics to a prostate tissue from the PCa patient with a high blood PSA level, and the PSAs were identified. After that, we intend to investigate PSAs in the tissue of PCa patient whose blood PSA level is in the gray zone of 4-10 ng/mL and compare the proteome of prostate cancer tissues also. Further study will be the targeted proteomics which captures only PSAs in PCa tissues.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 09:30

Chair: Sung Yul Lim (Kyung Hee University)

Assessment of health risk under exposure of airborne particulate matter in mouse by LC-MS based metabolomics

Seungwoo Seo, Tae-Young Kim*

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

In this study, liquid chromatography-mass spectrometry based metabolomics was performed on mouse model exposed to airborne particulate matter (PM). Exposure group mice were injected with PM by intratracheal instillation. Metabolites were extracted from the heart and the lung of exposure and control group mice. Partial least-squares discriminant analysis was conducted on the abundance of differentially expressed metabolites to examine whether exposure of PM caused difference in metabolite profiles between the two groups. Biological impact of PM exposure on mice was tracked by annotating metabolic pathways associated with differentially expressed metabolites. Common and unique biological implications between the two organs were also investigated, to evaluate total adverse effects on the cardiopulmonary system. This study suggested important metabolic changes resulting from PM exposure, which can be utilized to elucidate its toxicity mechanism.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 09:36

Chair: Sung Yul Lim (Kyung Hee University)

Synthesis and characterization studies of Mn and Co composite as a cathode material for lithium secondary batteries

Hyeseung Kwon, **Youngil Lee**[1,*]

University of Ulsan, Korea

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

$LiMBO_3$ (M=Mn, Fe, or Co), a polyanionic lithium metal borate as a cathode material for lithium secondary batteries, is actively being studied because of its light weight, structural stability, and high theoretical capacity (220 $mAhg^{-1}$). Among borate-based polyanionic materials, $LiMnBO_3$ has high operating potential, $LiCoBO_3$ has high operating voltage and high theoretical (215 $mAhg^{-1}$). Herein, monoclinic $LiMn_{1-x}Co_xBO_3$ (x = 0, 0.25, 0.5, 0.75, and 1.0) cathode materials have been synthesized by solid-state reaction method. X-ray diffraction (XRD) and solid-state ^7Li MAS NMR spectroscopy have been measured to characterize the crystal structure. Galvano electrostatic charge/discharge tests for prepared samples have been also studied to identify oxidation/reduction potential and operating voltage. Quantitative analysis of the chemical composition of the material has been also performed by laser-induced destructive spectroscopy (LIBS) and inductively coupled plasma-optical emission spectroscopy (ICP-OES).

Oral Presentation : **ANAL1.O-8**
Oral Presentation of Young Analytical Chemists I
Room 104 THU 09:42
Chair: Sung Yul Lim (Kyung Hee University)

Lipidomic analysis to evaluate effects of AMPK activation in diet-induced NASH mice

Yeajin Ju, Jueun Lee, Geum-Sook Hwang*

Western Seoul Center, Korea Basic Science Institute, Korea

Non-alcoholic steatohepatitis (NASH) is a risk factor for hepatocellular carcinoma accompanied by liver cell damage and inflammation along with fatty deposition. AMP-activated protein kinase (AMPK) plays an important role in controlling energy homeostasis and the activation can inhibit NASH pathology. However, the effect of the AMPK activation on hepatic metabolic rewiring is unclear. This study aimed to investigate the therapeutic effects of AMPK on hepatic metabolism on NASH using lipidomic analysis. C57BL/6J male mice were fed a choline-deficient high fat diet (CD-HFD) for 6 weeks to induce NASH and treated them with YE-21, a new direct AMPK activator candidate, every 2 days for 14 times. Then, we performed lipidomic profiling of liver tissue using ultra-performance liquid chromatography–quadrupole time-of-flight mass spectrometry. Mice were divided into four groups: control (n=12), YE-21 (n=12), CD-HFD (n=12), and CD-HFD+YE-21 (n=12). As a result of multivariate analysis, partial least squares-discriminant analysis (PLS-DA) score plots showed different lipidomic patterns between the CD-HFD and CD-HFD+YE-21 groups. Eleven and thirteen classes of lipid metabolites were identified in positive and negative mode, respectively. After YE-21 treatment, CD-HFD+YE-21 group, compared to CD-HFD group, had significantly higher levels of phosphatidylcholines (PCs) and phosphatidylethanolamines (PEs). In contrast, lower levels of diglycerides (DGs) and triglycerides (TGs) were observed in CD-HFD+YE-21 group than CD-HFD group. Interestingly, TGs with long acyl chains (>50 carbon atoms) were significantly increased in CD-HFD mice compared to control mice and then significantly decreased after YE-21 treatment, whereas there was no change in TGs with short acyl chins after YE-21 treatment. These data suggest that AMPK activation induces low levels of TGs, which were associated with steatosis amelioration. This study demonstrates that lipidomic analysis is effective method to investigate AMPK effects on NASH.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 09:48

Chair: Sung Yul Lim (Kyung Hee University)

Ionization behaviors and efficiencies of explosives of TNT, RDX, and PETN in APCI-MS

Chae eun Son, **Sung-Seen Choi**[1,*]

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

Explosives have been considered as most dangerous substances among the hazardous materials and they have property of exploding by friction or heat. 2,4,6-Trinitrotoluene (TNT), 1,3,5-trinitro-1,3,5-triazinane (RDX), and pentaerythritol trinitrate (PETN) are representative explosives, and they have been used as both of pure and blends form. Many reports represented that ionization efficiency of these explosive can be improved by chlorine dopants such as methylene chloride and chloroform. Mass spectrometry with electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) have been used to analyze explosives, but there are some complications that kinds of ions generated from the explosives vary depending on the solvent or the instrumental conditions. Principal ions produced from TNT by APCI are $TNT^{-\cdot}$ and $[TNT-H]^-$, those generated from RDX are $[RDX-H]^-$ and $[RDX+NO_2]^-$, and $[PETN-H]^-$ and $[PETN+NO_3]^-$ are the major ions of PETN. Especially, RDX and PETN can generate adducted ions with chloride, formate, or acetate. In this study, ionization behaviors and efficiencies of TNT, RDX, and PETN ionized by APCI were investigated using methylene chloride and acetone as the solvent. Analytical results could be explained using structures and energies of the product ions obtained by computational calculations.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 09:54

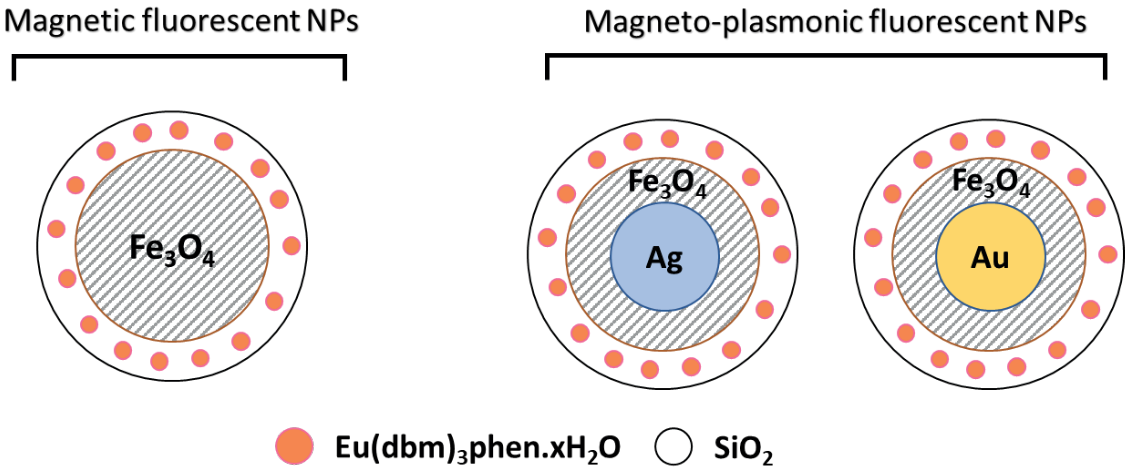
Chair: Sung Yul Lim (Kyung Hee University)

Rare earth doped Magnetoplasmonic nanoparticles for the detection of heavy metal ions in water

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

Department of Chemistry, Chungnam National University, Korea

Compared to fluorescent organic dyes or quantum dots, rare earth phosphors show superior luminescent lifetime, minimal photo-bleaching and enhanced biocompatibility. Moreover, the unique properties of the base nanoparticles such as magnetism or photonic effects could be utilized to enhance or modify the emission characteristics of the fluorophores. In this study, multifunctional RENPs based on magnetoplasmonic core-shell nanoparticles having both magnetic, plasmonic and photoluminescence properties were fabricated. The base magnetoplasmonic nanoparticles were synthesized using facile one-pot solvothermal methods, and doping of fluorescent rare-earth chelates using a modified sol-gel method were performed. The synthesized Eu-RENPs with Ag@Fe3O4 MagPlas NP cores shown enhanced photoluminescent emission intensities of over 50% compared to non-plasmonic MNPs doped systems, achievable by the local enhancement effect of the plasmonic core. The absolute quantum yield of the synthesized product reached as high as 30% by adjusting the Eu chelates doping ratio. Moreover, the synthesized MagPlas Eu-RENPs were utilized as a selective sensing probe for the determination of copper(II) ions in water. It is discovered that the energy transfer process to the localized transition metal ions, especially copper(II), resulted in the selective quenching of the fluorophore, which were highly proportional to the Cu2+ concentration in the range of (0.05 to 5 mg/L). The limit of detection and quantitation of this method fulfilled the requirements for determination of copper concentration in drinking water. Overall, magnetoplasmonic RENP probes are highly prominent for environmental monitoring, sensing and imaging applications.


Magnetic fluorescent NPs
Magneto-plasmonic fluorescent NPs
Fe_3O_4
Fe_3O_4
Ag
Fe_3O_4
Au
● $Eu(dbm)_3phen.xH_2O$
○ SiO_2

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 10:00

Chair: Sung Yul Lim (Kyung Hee University)

Characterizing the Optical Properties of Hollow Gold Nanoshells with Plasmonic Effect

Yun a Hong, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

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

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 10:06

Chair: Sung Yul Lim (Kyung Hee University)

Electrochemical biosensor for Influenza A H1N1 with multiple amplification strategy

Jonghwan Lim, Sanghyeon Park, Seunghun Kim, Eun Bin Kang, Wan Soo Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Multiple amplification strategy was devised for the improvement of the detection limit of electrochemical biosensor for influenza A. Electrochemical measurement by nanogap interdigitated electrode (nIDE) was combined with immunoassay using enzyme-linked polystyrene bead (PSB). Narrow gap in the nIDE facilitates the redox cycling of a probe molecule, giving an amplified electrochemical current, and the PSB increases the number of enzymes generating the probe molecule. In other words, the nIDE enhances the signal current at a fixed probe concentration, while the PSB raises the probe concentration at a fixed reaction time. As a result, limit of detection was extensively improved from 103 pM to 50 fM, compared to ELISA.

Oral Presentation : **ANAL1.O-13**
Oral Presentation of Young Analytical Chemists I
Room 104 THU 10:12
Chair: Sung Yul Lim (Kyung Hee University)

Synthesis of graphene oxide with highly preserved sp^2 carbon network as an efficient matrix for Laser Desorption/Ionization Time-of-Flight Mass Spectrometry

Seung-Woo Kim, Young-Kwan Kim[1,*]

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

Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) has been widely adopted for analyzing large molecular weight compounds such as peptides, proteins, nucleic acids and polymers. However, MALDI-TOF-MS cannot be applied directly to analysis of low molecular weight compounds due to the interference from the conventional matrix. Graphene oxide (GO) has been used as a matrix for matrix-free laser desorption/ionization time-of-flight mass spectrometry (LDI-TOF-MS) analysis to overcome this drawback. Unlike GO synthesized by Hummers' method (HGO), the commonly used in LDI-TOF-MS analysis, GO synthesized by modified Brodie's method (BGO) has highly preserved sp^2 carbon network and less defective structure. Here, we systematically compared HGO and BGO as a matrix for LDI-TOF-MS analysis of various analytes such as small molecules and synthetic polymers. The LDI mechanism on HGO and BGO was also explored by using a model thermometer molecule. Based on the results, we found BGO exhibited a much higher efficiency in LDI-TOF-MS analysis than HGO through the distinct LDI mechanism owing to its highly-preseved sp^2 carbon structures resulting in high laser energy absorption, photothermal conversion, thermal stability and conductivity.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 10:18

Chair: Sung Yul Lim (Kyung Hee University)

Recognition of bile components in bile using Au nanodendrite substrates modified with various alkanethiols as a tool for Raman spectroscopic identification of gall bladder cancer

Thu Thuy Bui, Hoeil Chung[*]

Department of Chemistry, Hanyang University, Korea

In gall bladder (GB), bile juice is stored and could be a valuable specimen for relevant GB disease diagnosis, since its composition would vary depends on pathological conditions of GB patients. Therefore, this study intends to investigate the potential for Raman spectroscopic discrimination of GB polyp and GB cancer using the aqueous phase samples extracted from 32 raw bile juice samples. Initially, an alkanethiol was conjugated to the surface of a SERS substrate (Au nanodendrite on Ni foil (AuND@NiF)) to generate SERS signal and attract bile components via mutual interaction. For more effective and thorough recognition of bile components, 4 independent substrates covered with 4 different alkanethiols with various functional groups ($SH(CH_2)_2CH_3$, $SH(CH_2)_2NH_2$, $SH(CH_2)_2COOH$, and $SH(CH_2)_2OH$) were prepared. When aqueous phase bile samples were measured using each substrate, varied SERS peaks in each case were mutually characteristics. When the principal component (PC) scores of spectra obtained using the $SH(CH_2)_2CH_3$- and $SH(CH_2)_2OH$-covered substrates were combined, the *k*-Nearest Neighbor based discrimination accuracy was 100%, superior to those (90.6-96.9%) using individual substrates. The use of complementary bile component-induced spectral information of these substrates was attributed to the superior discrimination performance.**Keywords:** Bile; Gall bladder cancer; Au nanodendrite; SERS

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 10:24

Chair: Sung Yul Lim (Kyung Hee University)

Synthesis and characterization of $LiFeBO_{3-x}F_{2x}/C$ nanocomposite as cathode material for Li-ion batteries

Yujin Son, Youngil Lee*

Department of Chemistry, University of Ulsan, Korea

Lithium iron borate ($LiFeBO_3$, LFeB) is considered as a promising cathode material for lithium-ion batteries (LIBs) because of its high theoretical discharge capacity of 220 mAh g^{-1}. However, LFeB cathode is limited to use in commercial LIBs by its low electrical conductivity resulting in low electrochemical performances. Fluorine substitution at the oxygen sites of LFeB to improve its low conductivity has been conducted with phase transition from monoclinic to vonsenite, in previous study. After the first charge/discharge cycle, however, the discharge capacity is significantly reduced. To overcome this problem, we have studied to improve the stability of its structure by carbon coating at the surface of F-doped $LiFeBO_3$(LFeBF) with maintaining high discharge capacity. The carbon-coated LFeBF (LFeBF/C) have been successfully synthesized by solid-state reaction method and characterized by X-ray diffractometry (XRD), SEM, TEM, and ^{7}Li MAS NMR spectroscopy. The electrochemical properties of LFeBF/C have been measured by using Galvano static charge/discharge test with the potential range of 1.0 - 4.5 V.

Oral Presentation : **ANAL1.O-16**
Oral Presentation of Young Analytical Chemists I
Room 104 THU 10:30
Chair: Sung Yul Lim (Kyung Hee University)

Quantitative proteomic analysis of VPA chemical mouse ASD model reveals enrichment of RNF146 and Wnt/ β-catenin signaling

Wooyoung Eric Jang, Min-Sik Kim[1,*]

Chemistry, Kyung Hee University, Korea
[1]*Department of New Biology, DGIST, Korea*

Autism spectrum disorder (ASD) is a heterogeneous neurodevelopmental disorder where patients have impaired social behavior and communication, repetitive behaviors, and restricted interests. While there have been numerous attempts to understand the pathogenesis of ASD, there is still no concrete understanding of ASD at a molecular level. We perform a global-relative-quantification analysis of the proteome of the VPA-induced ASD mouse model and control mouse's prefrontal cortex brain tissue. Relative quantification method by implementing TMT-labeled LC-MS/MS proteomic method, we observe a difference in proteomic level resulting in a better understanding of ASD in the molecular proteome. Our analysis shows that VPA-exposed mice showed up-regulation in upper neuronal regional proteins compared to the control. The proteomic data support the previous finding that ASD patients physically have more upper neurons. The overexpression or proliferation of neurons is directly related to the VPA chemical effect on prenatal brain development and Wnt/ β-catenin pathways. In this study, implementing proteomic approaches with network analysis revealed the molecular function of RNF146 related to ASD. Among the differentially expressed proteins, RNF146 (E3 Ubiquitin-protein ligase) increase in VPA exposed mouse showed a highly significant effect on canonical Wnt/ β-catenin signaling pathways the β-catenin beta-catenin destruction complex. The increase in RNF146 expression ubiquitinates AXIN protein, inhibiting the β-catenin destruction complex, resulting in decreased phosphorylated β-catenin. The proteins like CREBBP, TCF4, and GSK3B showed significant changes that indicate disfunction of β-catenin destruction complex and activation of transcription factors. Using the ASD mouse behavioral mouse test and western blot analysis have validated that RNF146 relation with ASD. This study contributes to understanding the proteome differences between ASD and control, and in our findings, RNF146 showed a clear indication of molecular correlation to ASD.

Oral Presentation : **ANAL1.O-17**
Oral Presentation of Young Analytical Chemists I
Room 104 THU 10:36
Chair: Sung Yul Lim (Kyung Hee University)

Identification of Secondary Organosiloxane Aerosol (SOSA) Using Aerosol Mass Spectrometry

Hwajin Kim

Environmental Health, Seoul National University, Korea

Volatile methyl siloxanes (VMS) are high-production chemicals emitted from many personal care products. Evidence from laboratory and ambient studies indicates that oxidized VMS products are present in particle phase and contribute to the formation of secondary organosiloxane aerosol (SOSA) . SOSA has most commonly been identified based on filter sampling and post-analysis. However, due to the low time resolution and time-consuming nature of offline methods, along with the sampling/storage artifacts, these methods are not ideal.In this work, we generated SOSA from oxidation of decamethylcyclopentasiloxane (D5, $C_{10}H_{30}O_5Si_5$) using an Aerodyne potential aerosol mass oxidation flow reactor (PAM OFR). The chemical composition of SOSA was characterized by high-resolution time of flight aerosol mass spectrometer (HR-ToF-AMS). In particular, we operated the instrument at an m/z range of up to ~1080 and for the first time observed a series of high-molecular ions of SOSA in the AMS mass spectra.Although the ability of AMS to characterize molecular composition is limited, the SOSA ions ($C_wH_xO_ySi_z$) can be identified by AMS. We also found the mass spectra from SOSA contained distinct groups of monomers, dimers and trimers, which reveals that the particles are composed mainly of products of D5 oxidation. The technique demonstrated here may offer new insights into characterizing SOSA related species and further can be used to identify the SOSA trace from ambient measurements both from indoor and outdoor.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 10:42

Chair: Sung Yul Lim (Kyung Hee University)

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

Seongeun Heo, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

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

Oral Presentation : **ANAL1.O-19**
Oral Presentation of Young Analytical Chemists I
Room 104 THU 10:48
Chair: Sung Yul Lim (Kyung Hee University)

The effect of water and heavy water on fibrillation dynamics of intrinsically disordered proteins

MyungKook Son, Chae Ri Park, Sooyeon Chae, Dongjoon Im, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Amyloid proteins undergo self-assemblies to form insoluble fibrillar aggregates with a highly ordered □-sheets. These fibrils are associated with various human diseases, known as amyloidosis. To study amyloid-associated protein dynamics, various spectroscopic techniques such as Nuclear Magnetic resonance (NMR) spectroscopy, Infrared (IR) spectroscopy, etc. are utilized for the structural analysis. To avoid spectroscopic peak interferences such as H resonance frequency or O-H vibrational frequency in NMR and IR spectroscopy, deuterium oxide (D2O) is commonly used as a solvent for a deuteration of sample molecules. However, due to isotope effect of D2O, hydrogen bonding and hydrophobic effect are known to have stronger effect compared to H2O. Recently, we have found that D2O stabilize the folding structures of insulin, due to enhanced H-bonding and hydrophobic effect, inhibiting the fibrillation of insulin. In this research, we used α-synuclein and K18 to study the effect of reinforced hydrophobic effect on the intrinsically disordered protein (IDP) structures and protein stability-fibrillation. Small angle X-ray scattering (SAXS) and ion mobility mass spectrometry (IM-MS) were utilized for the study of solution phase and gas phase initial protein structures, and thioflavin-T (ThT) assay, circular dichroism (CD) and transmission electron microscopy (TEM) were utilized to compare the fibrillation kinetics in H2O and D2O.

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

Oral Presentation of Young Analytical Chemists I

Room 104 THU 10:54

Chair: Sung Yul Lim (Kyung Hee University)

Rapid and sensitive detection of SARS-CoV-2 using SERS-based microdroplet sensor

Sohyun Park, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

The coronavirus disease 2019 (COVID-19) has been labeled an ongoing pandemic by the World Health Organization (WHO). Real-time quantitative polymerase chain reaction (RT-qPCR) has been considered a gold standard for the quantitative evaluation of a target gene. However, it still suffers from the problem of a long detection time. Commercially available lateral flow assay kits can be taken within 30 min, but it has low sensitivity and poor accuracy problems. To address these issues, we developed a surface-enhanced Raman scattering (SERS)-based immunosensing platform for the rapid and sensitive detection of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). In this work, SERS nanoprobes, which are anti-SARS-CoV-2 nucleoprotein antibody-conjugated gold nanoparticles, and magnetic beads have been used to detect SARS-CoV-2 nucleoprotein. The Raman signals of SERS nanoprobes for magnetic immunocomplexes were measured under flowing conditions inside a microdroplet channel. Total analysis time from droplet generation to SERS detection takes less than 10 minutes because all experimental conditions were automatically controlled inside the exquisitely designed microfluidic channel. This novel SERS-based immunosensing platform using a microdroplet channel is expected to be a powerful analytical tool to detect SARS-CoV-2.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 09:00

Chair: Hyun Hee Lee (Korea Food Research Institute)

Optically tunable plasmonic chiral superstructure

Siyeong Hwang, Juyong Gwak[1], Jaebeom Lee[2,*]

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

2D metasurfaces have engaged enormous academic attention from their properties of manipulating polarized light and relatively facile fabrication. A new facile fabrication method for 2D chiral metasurface using magnetic field-induced nanoarray was proposed herein to make amend of current 2D metasurfaces and to develop dynamic in-situ tenability. The tunability of a chiroptical response was certified through adjustments of the curvature applied to the substrate. The application of the curvature induced a skew angle which is an angle between pattern direction and curvature, and it broke the symmetry of the structure which resulted in chirality. When the skew angle got closer to ±45°, a circular dichroism spectrum intensity got bigger which means the chiral response was enhanced. This extremely facile fabrication approach to magnetic self-assembly nanoarray inspires possibilities of mass production and a wide-range detection.

Oral Presentation : **ANAL2.O-2**
Oral Presentation of Young Analytical Chemists II
Room 104 FRI 09:06
Chair: Hyun Hee Lee (Korea Food Research Institute)

SERS-LFA strip for rapid classification of Influenza A and SARS-CoV-2

Mengdan Lu, Jaebum Choo[1,*]

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

The spread of COVID-19 has caused enormous economic and social losses worldwide. In addition, there is a prediction that there may be a flu epidemic at the same time this fall. Since influenza and COVID-19 have similar symptoms such as fever, cough, sore throat, muscle aches, and diarrhea, it is essential to quickly determine whether a suspected patient is infected with COVID-19 or Influenza to prevent the spread of COVID-19 effectively. Although a rapid immunochromatic kit has been commercialized for this purpose, it has low diagnostic reliability due to the false-negative issue and low sensitivity. To solve this problem, we developed a highly sensitive SERS-based lateral flow assay (LFA) strip that can detect influenza virus (H1N1) and COVID-19 simultaneously with high accuracy. According to our assay results, the limits of detection (LoDs) for influenza a virus (H1N1) and SARS-CoV-2 were 57 HAU/mL and 4 PFU/mL, respectively. These values are approximately 500 times more sensitive than those measured from commercially available rapid LFA kits.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 09:12

Chair: Hyun Hee Lee (Korea Food Research Institute)

Investigation of TPT-VCR multidrug mechanisms in 3D spheroids human neuroblastoma cells

Sooyeon Chae, Chae Ri Park, MyungKook Son, Dongjoon Im, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Neuroblastoma is a common extracranial solid tumor in childhood, which begins when immature nerve cells grow out of control in the adrenal gland, abdomen, pelvis, chest, and neck. Multidrug regimen chemotherapy has been underway to optimize therapeutic outcomes, maximize treatment efficiency. The multidrug regimen with topotecan and vincristine was used for neuroblastoma patients. Topotecan (TPT) is an anti-tumor drug that forms a ternary complex into [topoisomerase I-DNA-TPT], preventing DNA replication. Vincristine (VCR) is also an anti-tumor drug, and its mechanism of action is interaction with tubulin to inhibit mitosis. Several clinical tests showed that the multidrug regimen with TPT and VCR have synergistic toxicity. However, the specific mechanism of this effect is still ambiguous due to challenges at mimicry of pharmacokinetics and the tumor microenvironment at the laboratory level. In this study, we aim to investigate TPT-VCR multidrug mechanisms and mimic pharmacokinetics and tumor microenvironment. 3D spheroid SK-N-SH neuroblastoma cells treated with TPT and VCR multidrug showed a synergistic effect compare to single-drug treatment. The tubulin polymerization data showed that the action of vincristine was reduced in multidrug treatment, which implies another pathway for a synergistic effect. For more detailed investigation, we plan to mimic pharmacokinetics and tumor microenvironment using A fluidic system.

Oral Presentation : **ANAL2.O-4**
Oral Presentation of Young Analytical Chemists II
Room 104 FRI 09:18
Chair: Hyun Hee Lee (Korea Food Research Institute)

Investigation of Oxygen Plasma Treatment Effect on Au@AuHg alloy Nanoparticles

Jaeran Lee, **Ji Won Ha***

Department of Chemistry, University of Ulsan, Korea

This study shows oxygen plasma treatment effect of Au@AuHg alloy core-shell nanoparticle for the structural, localized surface plasmon resonance (LSPR) spectral, and surface Au atom distribution changes. Au@AuHg alloy nanoparticles subjected to different plasma treatment times were characterized using transmission electron microscopy (TEM) and total internal reflection scattering(TIRS) microscopy and spectroscopy. The mercury ion solution treatment for 3 hours changed AuNR to Au@AuHg alloy spherical particles, and the thickness and atomic ratio of the shell and core was confirmed through TEM. The AR of the single Au@AuHg alloy was decreased by structural deformation, while their LSPR linewidth was increased with increasing plasma treatment time. But the three-dimensional (3D) orientations of the particle showed non-variation tilt angles with oxygen plasma treatment . The results show that the shape of the AuHg alloy shell deformed close to spherical shape through oxygen collision, but did not induce deformation of the Au core in the process of the oxygen plasma treatment. Therefore, this study provides a deeper understanding of energy transfer distance by oxygen collision through plasma treatment of Au amalgam shell nanoparticles.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 09:24

Chair: Hyun Hee Lee (Korea Food Research Institute)

Synthesis of $LiFe_{1-x}Mn_xBO_{2.7}F_{0.6}$ as a cathode material for Li-ion battery

Daeun Han, **Youngil Lee**[*]

Department of Chemistry, University of Ulsan, Korea

Among the cathode materials of lithium-ion batteries, borate-based materials have been studied a lot so far due to their high theoretical capacity (220 mAh g^{-1}). One of these borate-based materials, $LiFeBO_3$ has good stability, low open-circuit voltage (OCV), and good reversible capacity. In a previous study, we have shown that the discharge capacity of $LiFeBO_{2.7}F_{0.6}$ has been improved by doping fluorine into $LiFeBO_3$. However, structural instability has been observed. Therefore, in this study, manganese is added to the metal site of $LiFeBO_{2.7}F_{0.6}$ to acquire its structural stability. $LiFe_{1-x}Mn_xBO_{2.7}F_{0.6}$ (x = 0, 0.25, 0.5, 0.75 and 1.0) have been synthesized by solid-state method and characterized their structure by ^7Li MAS NMR and X-ray diffraction (XRD). The stability of the structure has also been verified by measuring the electrochemical performances with the Galvano static charge-discharge test.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 09:30

Chair: Hyun Hee Lee (Korea Food Research Institute)

Efficacy of Natural Antibacterial Feed in Paralichthys Olivaceus using Proteomics

Junghoon Kang, Youngjin Kim, Wonryeon Cho*

Department of Chemistry, Wonkwang University, Korea

Antibiotics and chemotherapeutics have been frequently used to treat bacterial infection in order to prevent mass mortality in aquaculture products such as Paralichthys olivaceus (P. olivaceus). However, these compounds may eliminate beneficial bacteria and produce antibiotic-resistant pathogenic strains, and thus remain as residues in the human body. This study aims to analyze the efficacy of antibacterial feed by detecting proteome alteration of P. olivaceus after feeding antibacterial feed, which is being developed using natural amino acids generated from animals and plants. One group of P. olivaceus was fed antibacterial feed while another group was fed general feed for four weeks, and then both groups were artificially infected with Streptococcus parauberis. Proteins were extracted with RIPA buffer from homogenized head kidney tissues of both P. olivaceus groups. Then each supernatant fluid was trypsin digested and desalted respectively. After that, the proteins in both groups were identified with nLC-MS/MS and protein database searches. Proteins were significantly identified only in the group fed with antibacterial feed, and the efficacy of the antibacterial feed was analyzed by performing protein functional analysis.

Oral Presentation : **ANAL2.O-7**
Oral Presentation of Young Analytical Chemists II
Room 104 FRI 09:36
Chair: Hyun Hee Lee (Korea Food Research Institute)

Long-term Effects of Exposure to Microplastics at Environmentally Relevant Concentrations on Lipidome of the Mouse Heart and Brain

Jonghyun Kim, Tae-Young Kim[*]

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

Most studies on the toxicological effects of microplastics (MPs) have been limited to a relatively short-term duration under high concentrations which are irrelevant to human exposure conditions. To overcome the limitation, this study investigated the long-term effects of MP exposure at environmentally realistic concentrations on the mouse cardiac and brain lipidome. The concentrations of MPs were determined based on the reported abundances of MPs in foods and their daily consumptions. In the consideration of size-dependent absorption of MPs through the digestive system, only MPs with size less than 10 μm were exploited for the experiments. MPs were orally administered to mice via drinking water for 1, 3, and 6 months. Relative quantification of lipids was carried out by deuterium oxide labeling for global omics relative quantification (DOLGOReQ). To reveal the relationship between quantitative change of lipids and the exposure conditions including exposure period, size, and polymer type of MPs, statistical analysis using ANOVA for the exposed groups was performed. Our results implied that the reported toxic effects of MPs could have been overestimated due to the use of excessively high concentration of MP.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 09:42

Chair: Hyun Hee Lee (Korea Food Research Institute)

Lipidomic profiling in serum and liver tissue of mice with nonalcoholic steatohepatitis (NASH)

Jiaxin Geng, Youngae Jung[1], Geum-Sook Hwang[1,*]

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

Nonalcoholic fatty liver disease (NAFLD) has become a global health problem, affecting 25% adult population. NAFLD is a spectrum disease ranging from simple steatosis, to nonalcoholic steatohepatitis (NASH) and hepatocellular carcinoma (HCC). However, there is still not enough data for lipid alteration in the process of NASH. In this study, we examined the lipidomic changes in serum and liver tissue of mice (n=16) using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC/QTOF-MS). Control and NASH groups were fed with chow diet (n=8) and NASH diet (n=8) for 3 weeks, respectively. Score plots derived from principal component analysis (PCA) showed separations between control and NASH groups. Total 14 classes of lipids were identified from LC-MS data and then Mann-Whitney test was used to show the alterations of lipids in serum and liver tissue. Free fatty acids (FFAs) such as poly unsaturated FAs (PUFAs) showed similar decreases in both serum and liver tissue in NASH group. On the other hands, phospholipids and glycerolipids differed in NASH group between serum and liver tissue. This study demonstrates that UPLC-MS/MS based lipidomic profiling is a useful tool in detecting characteristic changes at early stages of NASH in serum and liver tissue.

Oral Presentation : **ANAL2.O-9**
Oral Presentation of Young Analytical Chemists II
Room 104 FRI 09:48
Chair: Hyun Hee Lee (Korea Food Research Institute)

A Study on the Effect of Ammonium ions on Yb/Lu Separation Efficiency

Aran Kim, Kang Hyuk Choi*

Radioisotope Research Division, Korea Atomic Energy Research Institute, Korea

The no-carrier added (nca) lutetium-177 (^{177}Lu, $t_{1/2}$ = 6.7 d) are a promising therapeutic radionuclide in nuclear medicine because it has high specific radioactivity and high radionuclide purity without long-lived radioactive impurity. The nca ^{177}Lu can be produced via the ^{176}Yb(n,γ)^{177}Yb → ^{177}Lu reaction, where the process of separating it from a macroscopic amount of Yb target is important. Ion exchange chromatography is generally used to separate two adjacent nuclides Yb and Lu, with α-HIBA (α-hydroxyisobutyric acid) as complexing agent and NH_4^+ (ammonium hydroxide) as separating ion. Numerous papers evaluating the separation efficiency have studied the effect of the concentration of the eluent, but few papers have evaluated the separation efficiency using separating ion other than normal NH_4^+ ion. Thus, in this study, the separation efficiency of stable isotopes Yb and Lu was evaluated by using different ammonium ions, including primary, secondary and tertiary ammonium ions, replacing NH_4^+ ion. Separation experiments were carried out using α-HIBA with pH adjusted using ammonium hydroxide, methylamine, ethylamine, diethylamine, pyridine, ethanolamine and ethylenediamine, respectively. Since the column retention time and elution time increase as the amine order increases, it is important to select an appropriate type of ammonium ion for effective and selective separation of Yb and Lu.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 09:54

Chair: Hyun Hee Lee (Korea Food Research Institute)

Maximization of chiral chromatography efficiency through temperature control

Danbi Eun, Jae Jeong Ryoo[1,*]

Dept. of Chemistry Education, Kyungpook National University, Korea
[1]*Department of Chemical Education, Kyungpook National University, Korea*

The separation of two enantiomers is very important in many scientific fields.[1] If the enantiomers are separated and the two separated peaks are far apart, it is because the interaction between the two enantiomers of sample and the chiral selector (stationary phase material in the chiral column) is good and shows a large separation factor value. In addition, when the base line of the two peaks of the separated enantiomers is clearly separated, it shows a large resolution value, is effective for mass separation of chiral compounds, and it is advantageous to obtain optically pure chiral compounds from a practical point of view.In this study, how effectively the separation was changed in terms of separation factor (a) and resolution (Rs) through manual temperature control in the separation of two enantiomers of a racemic mixture for five chiral compounds[2,3] (N-3,5-DNB-DL-Leucine, N-3,5-DNB-DL-Alanine, N-3,5-DNB-DL-Phenylalanine, N-3,5-DNB-DL-Valine, N-3,5-DNB-DL-Phenylglycine) using HPLC. Through this study, it was confirmed that the analysis efficiency can be significantly increased through simple heating/cooling in HPLC.[1] Ward TJ, Ward KD. Chiral separations: a review of current topics and trends. Anal Chem 2012;84:626–635.[2] Yu JJ, Ryoo DH, Lee JM, Ryoo JJ. Synthesis and Application of C2 and C3 Symmetric (R)-Phenylglycinol-Derived Chiral Stationary Phases. Chirality 2016;28:186-191.[3] Ryoo JJ, Kim TH, Im SH, Jeong YH, Park JY, Choi SH, Lee KP, Park JH. Enantioseparation of racemic N-acylarylalkylamines on various amino alcohol derived π-acidic chiral stationary phases. J Chromatogr A 2003;987:429-438.

Oral Presentation : **ANAL2.O-11**
Oral Presentation of Young Analytical Chemists II
Room 104 FRI 10:00
Chair: Hyun Hee Lee (Korea Food Research Institute)

Dynamic Nuclear Polarization of Selectively 29Si Isotope-Enriched Silica Nanoparticles

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

Department of Bionano technology, Hanyang University, Korea
[1]*Department of Bionano Technology, Center for Bionano intelligence Education and Research, Hanyang University, Korea*
[2]*Department of Applied chemistry, Hanyang University, Korea*
[3]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*
[4]*Department of Bio-Nano Engineering, Department of, Korea*

Silica nanoparticles have garnered attention as promising biomedical probes for hyperpolarized 29Si magnetic resonance imaging and spectroscopy. We have demonstrated a straightforward method of synthesizing selectively 29Si enriched nano-sized silica particles with high degrees of control in terms of the particles' physicochemical properties and size. By utilizing 100% 29Si enriched TEOS, a silica precursor, selective enrichments on either particle surface (10 nm thickness) or core (40 nm diameter) were precisely conducted. With the particles of various structural characteristic, dynamic nuclear polarization (DNP) properties ranging from buildup, enhancement factor, and depolarization time at a cryogenic temperature were examined. The best considerable signal amplification was achieved from the silica nanoparticle with a selective enrichment localized on the particle surface, exposing both the successive surface polarization and polarization profile. The synthetic strategy with selective enrichments on the particles may expand the practical applicability of the nano-sized silica materials in various biomolecular processes, including targeted molecular imaging in vivo.

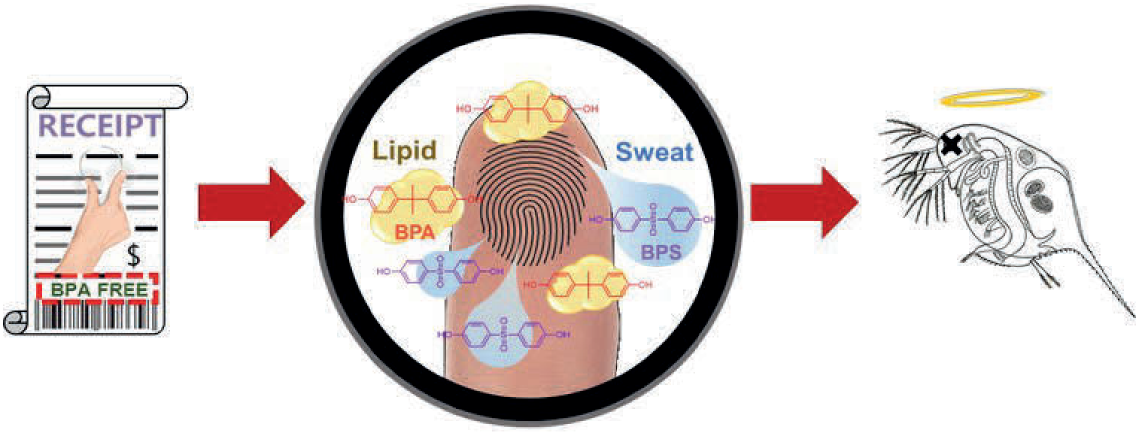
Oral Presentation : **ANAL2.O-12**
Oral Presentation of Young Analytical Chemists II
Room 104 FRI 10:06
Chair: Hyun Hee Lee (Korea Food Research Institute)

The risk of dermal exposure of BPA-free materials

Min Jang

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

Bispheonl A (BPA) is still being found in a wide array of manufactured products including thermal papers, plastic water bottles, canned foods, and pacifiers despite reported toxicity of BPA to human beings. BPA is also a frequently used monomer in engineering plastics. Therefore, consistent requests of BPA replacement have been surged. Bisphenol S (BPS) is one of replacements and BPS containing materials (receipts and colored papers) are sold in the market labeled as BPA-free. However, is it actually safe?This research reported that BPS is present in BPA-free labeled materials with enormous amount (10000 and 500 μg/g, respectively). Since they are handled by human beings in daily basis, BPS can be transferred to human skin. Our newly developed liquid chromatography mass spectrometry (LC-MS) method qualitatively and quantitatively detected BPS (5 to 26 μg/g) as well as BPA (28 to 89 μg/g) in fingerprints. Furthermore, using a matrix assisted laser desorption ionization mass spectrometry image (MALDI-MSI) method confirmed visually the presence of BPS in a fingertip after a receipt handled, and that presence of sufficient oily materials without handwashing can pick up more amount of BPS than with handwashing. The level of BPS in fingerprints was then applied to the toxicity test using water flea. As a result, chronic exposure to BPS in spite of low concentration still adversely influenced on the birth and health of water flea. It means that chronic handle of BPA-free materials can be a big threat to the health system.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Oral Presentation : **ANAL2.O-13**

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 10:12

Chair: Hyun Hee Lee (Korea Food Research Institute)

Engineering and Identification of Marine Bioactive Peptide to Enhance the Properties of Antioxidant and Anti-inflammatory

Soyun Choi, Dong-Ku Kang*

Department of Chemistry, Incheon National University, Korea

It has been discovered that various marine active peptides have antioxidant and anti-inflammatory activities. QHGV (glutamine-histidine-glycine-valine), oyster-derived peptide has been widely investigated its' anti-aging and anti-inflammatory functions. Here, QHGV peptide is modified by adding various naturally-derived phenolic acids, which has C-3 methoxy radicals or C-4 hydroxyl in aldehyde or benzyl alcohol. Five types of phenolic acids are selected to provide superior antioxidant effects and phenolic acids were conjugated at the end of N-terminus. Cellular ROS was more decreased by Phenolic acid-conjugated QHGV comparing non-modified QHGV and phenolic acid conjugated does not induce cellular toxicity in HaCaT cells. In addition, Phenolic acid induces collagen expression of mRNA and protein level in HaCaT cells. It has been also well-identified that oxidative-stress relates with inflammatory responses. Therefore, effect of phenolic acid conjugation was characterized on anti-inflammatory property of QHGV peptide. Results indicate that phenolic acid conjugation inhibits LPS-induced nitric oxide synthase (iNOS) and cyclooxygenase-2 (COX-2) in mRNA level. These results suggest that modification of phenolic acid provides additional and stronger biological activities on QHGV peptides.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 10:18

Chair: Hyun Hee Lee (Korea Food Research Institute)

Identification and Analysis of Biomarkers from Novichok-inhibited Human Plasma

Woo-Hyeon Jeong

Chem-Bio Technology Center, Agency for Defense Development, Korea

NOVICHOK is a series of novel nerve agents reported firstly in Skripal Attack in 2018. We identified biomarkers from Novichok-inhibited human plasma for verification purposes. Butyrylcholinesterase and Human Serum Albumin were chosen for the target of biomarker identification using protease digestion and estimated the structure and exact mass of Novichok-inhibited biomarkers based on finding for conventional nerve agents. We successfully detected biomarkers for verification against Novichok in human plasma, and their MS2 Spectra was assigned and utilized for further analysis of OPCW Biomedical Proficiency Test (BioPT) or authentic plasma samples.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 10:24

Chair: Hyun Hee Lee (Korea Food Research Institute)

Colorimetric Detection for Receptor Binding Domain of SARS-CoV-2 virus for Developing Paper-based Immunoassay

Xiaoyue Xu, In Geol Choi[1,*]

Department of Biotechnology, Korea University, China
[1]*Department of Biotechnology, Korea University, Korea*

AbstractSince the COVID-19 caused an outbreak in December 2019, millions of people in the world have been infected with the virus because of its high speed of transmission and the number of infections is still increasing, regardless of vaccination. The most common diagnostic method used in clinics is RT-PCR because it is the most accurate method but time-taking. Fast, simple, accurate and self-available diagnostic methods have been explored constantly to avoid infection. To develop a Do-It-Yourself (DIY)) diagnostic kit, paper-based colorimetric immunoassay was considered. This method is based on the interaction between antigen (RBD of SARS-CoV-2) and antibody (H11-D4). We employed Aryl Acylamidase (AAA) as a reporter that gives a color change. We cloned and overexpressed an antibody protein fused with AAA (H11-D4-AAA) to bind the spike protein of SARS-CoV-2. The binding affinity of H11-D4-AAA against RBD was determined as 131nM using surface plasmon resonance and the detectability also confirmed by dot blot assay. The detection limit of this colorimetric method was lower sensitivity than RT-PCR when the image analysis was applied (e.g. photographing using smartphone).Keywords: DIY, paper-based colorimetric immunoassay, SARS-CoV-2, aryl acylamidaseAcknowledgmentThis work was supported by Center for Women In Science, Engineering and Technology(WISET) grant funded by the Ministry of Science and ICT(MSIT) under the team research program for female engineering students.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 10:30

Chair: Hyun Hee Lee (Korea Food Research Institute)

Synthesis and characterization of iodine-doped $LiFeBO_3$ as cathode for lithium-ion battery

Yujin Jeong, Youngil Lee[*]

Department of Chemistry, University of Ulsan, Korea

Among the types of cathode material for lithium-ion batteries, polyanionic compounds have higher thermal stability and better safety properties due to the strong covalent bond of oxygen atoms, which make them more suitable for large-scale applications of lithium-ion battery. Among iron-based polyanion compounds, LFeB ($LiFeBO_3$) is a promising cathode material because it has the lowest weight framework and provides a high theoretical capacity of 220 mAh/g. Therefore, there are various studies on anion-doping as a method to improve the poor electrical conductivity of LFeB. So herein, doping of iodine, a relatively less study in cathode materials, has been conducted. For iodine-doped LFeBI ($LiFeBO_{3-x}I_{2x}$), it is important to set an appropriate synthesis temperature because of the rapid sublimation of iodine. XRD measurement has been performed to confirm the phase change of LFeBI depending on doping ratio synthesized by solid-state reaction, and electrochemical performance evaluated to confirm the improvement of electrical conductivity.

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

Oral Presentation of Young Analytical Chemists II

Room 104 FRI 10:36

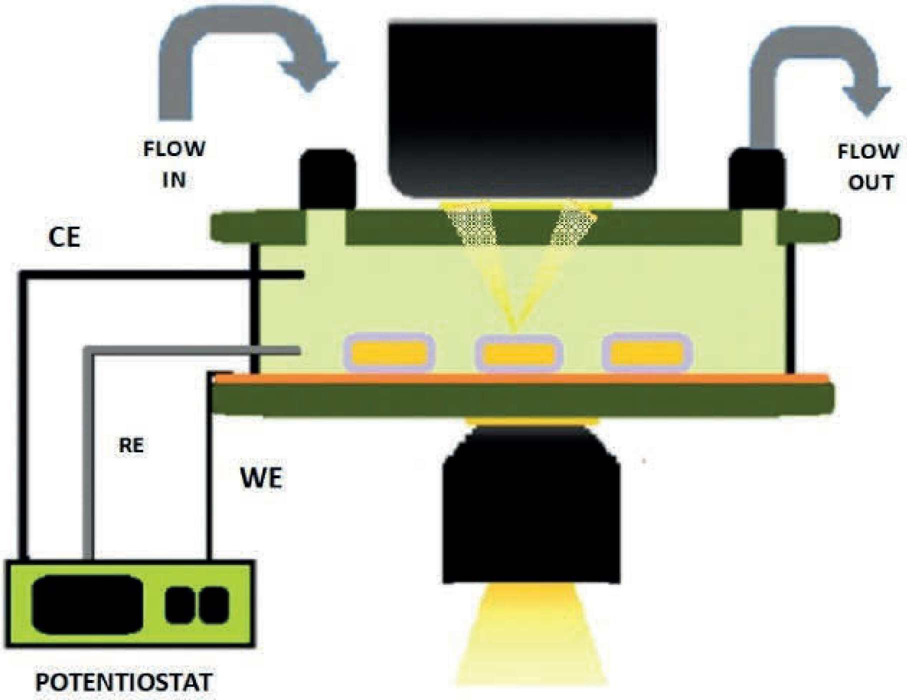
Chair: Hyun Hee Lee (Korea Food Research Institute)

Characterizing Mercury Amalgamation on Single Mesoporous Silica Coated Gold Nanorods Using Spectroelectrochemistry

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

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

Direct observation of chemical reactions in metallic nanoparticles is of great importance to have a deeper understanding of these processes for their uses in nanoparticle-based sensing and catalytic applications. Recently, scattering-based dark-field (DF) microscopy has been incorporated into electrochemical cells for enabling optical investigation of electrochemical processes on nanoparticle surface (Figure 1). In this spectroelectrochemical approach, electrodes constituted by low-density nanoparticles deposited on ITO substrates were used to inject electrons into nanoparticles whose optical response was then monitored by DF microscopy. In the present study, we used spectroelectrochemistry (electrochemistry + DF microscopy and spectroscopy) to characterize mercury amalgamation on gold nanorods coated with mesoporous silica shell (AuNRs@mSiO_2O) at the single particle level. Mercury (Hg^{2+}) was electrochemically reduced at AuNR electrodes, and the consequent optical changes resulting from deposition of mercury were monitored by scattering-based DF microscopy. Mesoporous silica shell allowed for approaching of mercury on the AuNR surface. Single AuNRs@mSiO_2O showed longitudinal surface plasmon resonance (LSPR) blue-shifts as well as a linewidth broadening in their scattering spectra, caused by the reduction (or amalgamation reaction) of mercury on the Au nanoparticle surface. Furthermore, reduction peaks were observed at potentials which were attributed to Hg^{2+} reduction under linear sweep voltammetry.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Oral Presentation : **ANAL2.O-18**
Oral Presentation of Young Analytical Chemists II
Room 104 FRI 10:42
Chair: Hyun Hee Lee (Korea Food Research Institute)

Comparing equilibrium structures of the Amyloid-β (1-42) dimers and assembly properties *in vitro*

Dongjoon Im, MyungKook Son, Chae Ri Park, Sooyeon Chae, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Senile plaque of Amyloid-β (1-42) is well-known pathological hallmark in Alzheimer's disease. High aggregation propensity is a major characteristic of Amyloid-β (1-42). In the previous study, we investigated equilibrium ensembles of Amyloid-β (1-42) on the basis of 19.2 μs replica exchange molecular dynamics simulations (400 ns per replica). From this simulation results, we confirmed that hydrophobic interaction plays a pivotal role in the self-assembly process of Amyloid-β (1-42) and contacts between side chains occur frequently in the specific domain. We also observed that substitution of the hydrophobic core residues into hydrophilic amino acid decelerates its fibrillation process. Herein, we obtained equilibrium ensembles of mutant peptide homo dimer and hetero dimer with wild type. To further investigation of inter-molecular states, we performed Markov State Model analysis. The free energy landscape of mutant peptide has multiple local minima whereas the wild type had only one global minimum state. Combined with mass spectrometry analysis, we can understand the underlying mechanisms in kinetical delay of the self-assembly process of Amyloid-β (1-42) with its point mutant.

Oral Presentation : **ANAL2.O-19**
Oral Presentation of Young Analytical Chemists II
Room 104 FRI 10:48
Chair: Hyun Hee Lee (Korea Food Research Institute)

SERS-PCR Assays of SARS-CoV-2 using Au nanoparticles-inserted Au nanodimple substrates

Yixuan Wu, Jaebum Choo[1,*]

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

The reverse transcription-polymerase chain reaction (RT-PCR) method has been adopted worldwide to dignose severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Although this method has good sensitivity and specificity, there is clearly a need to develop a more rapid diagnostic technology, given the virus's rapid spread. However, the RT-PCR method takes a long time to diagnose SARS-CoV-2 because of the required thermocycling steps. Therefore, we developed a surface-enhanced Raman scattering (SERS)-PCR detection method using an AuNP-inserted Au nanodimple substrate (AuNDS) to shorten the diagnosis time by reducing the number of thermocycling steps needed to amplify the DNA. For the envelope protein (E) and RNA-dependent RNA polymerase (RdRp) genes of SARS-CoV-2, when the initial DNA concentration was 1.00 × 10^5 copies/μL, 25 RT-PCR thermocycles are required to reach a detectable threshold value, while 15 cycles are required for magnetic bead-based SERS-PCR. However, only 8 cycles are needed for the AuNDS-based SERS-PCR, and the corresponding detectable target DNA concentrations were 3.36 × 10^12, 3.28 × 10^9, and 2.56 × 10^7 copies/μL, respectively. Therefore, AuNDS-based SERS-PCR is seen as being a new molecular diagnostic platform that can shorten the time required for the thermocycling steps relative to the conventional RT-PCR.

Award Lecture in Division : **LIFE.O-6**
Oral Presentations by Young Life Chemists
Room 105 THU 10:10
Chair: Hak Joong Kim (Korea University)

Generation of biomolecular diversity: molecular logic and application

Seokhee Kim

Division of Chemistry, Seoul National University, Korea

Biomolecular diversity underlies not only the complexity of biological systems, but the adaptation and evolution of organisms in a new environment. The living organisms, therefore, have developed sophisticated mechanisms to generate and manipulate diverse biomolecules. By using approaches in molecular biology, bioinformatics, enzymology, and structural biology, my research aims at dissecting various aspects of the generation of biomolecular diversity, and exploiting these Nature's processes for practical applications. One goal of my research is to expand the natural scope of a class of natural products, ribosomally-synthesized and post-translationally modified peptides (RiPPs), and to dissect the biosynthetic pathway and mechanism. In contrast to non-ribosomal peptides and polyketides that share several common biosynthetic enzymes, RiPPs are synthesized by a much diverse set of primary modification enzymes. Therefore, it is still unknown how many novel RiPPs exist in nature. This research currently focuses on multicyclic peptides with ester/amide crosslinks (OEPs or graspetides). Another research aims at developing a new approach of directed evolution of proteins. Directed evolution mimics the process of the natural protein evolution to obtain better variants in laboratory. However, traditional directed evolution relies on in vitro DNA diversification, and thus, is limited by labor-intensive discrete steps and relatively low size of DNA library. Our group is developing novel in vivo mutagenesis methods with high target-specificity and applying them to the evolution of enzymes of practical value. These studies will ultimately help explore novel structural and functional space of biomolecules with implications in biotechnology and medicine.

Oral Presentation : **LIFE.O-1**
Oral Presentations by Young Life Chemists
Room 105 THU 09:00
Chair: Woon Ju Song (Seoul National University)

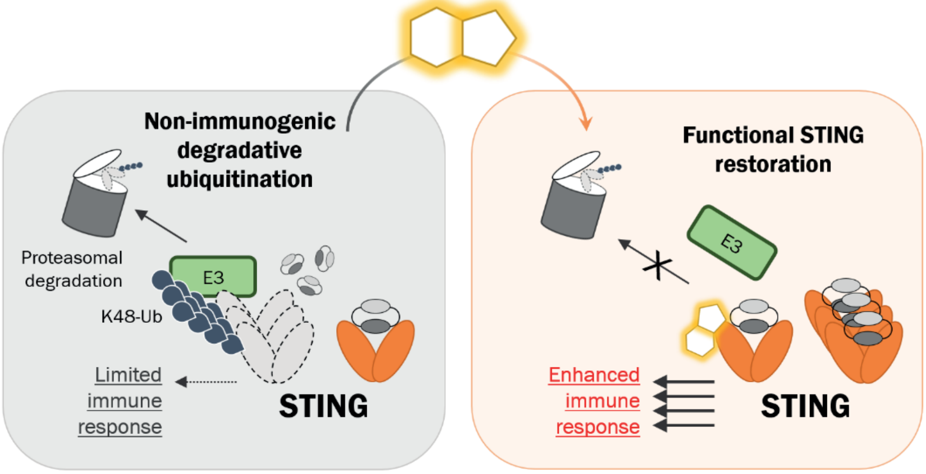
A targeted protein upregulation strategy potentiates STING agonists in cancer immunotherapy

Wansang Cho, Seung Bum Park[1,*]

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

As cancer immunotherapy has been emerged as a new pillar of cancer therapy, many strategies modulating host immunity were suggested for cancer treatment. Stimulator of interferon genes (STING) is a promising target for anticancer immunotherapy. However, dysregulated STING expression, or poor pharmacokinetic profiles of STING agonists pose major challenges. Recently, modulating target protein levels via the ubiquitin-proteasome system, such as proteolysis-targeting chimera (PROTAC), has broadened the scope of pharmacological inventions. Herein, we propose UPPRIS (upregulation of target proteins by protein-protein interaction strategy) to overcome these limitations. We discovered the small molecule SB24011 that inhibits STING–E3 ligase interaction, thereby induces the blockade of E3 ligase-mediated STING degradation. As a result, SB24011 enhanced the STING agonist-mediated immune responses by upregulating cellular STING protein level. Thus, co-administration of SB24011 markedly improved the immuno-oncological efficacy of STING agonist cGAMP and anti-PD-1 therapy for tumor regression and robust systemic antitumor response. Taken together, we successfully demonstrated that targeted STING protein upregulation is a promising strategy for cancer immunotherapy.

UPPRIS: Upregulation of target proteins by protein-protein interaction strategy



STING downregulation by
E3 ligase-mediated degradation
Limited STING agonist activity

Targeted STING upregulation by
blocking STING-E3 ligase interaction
Enhanced STING agonist activity

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

Oral Presentations by Young Life Chemists

Room 105 THU 09:12

Chair: Woon Ju Song (Seoul National University)

A genetically encoded fluorescent sensor for protein Arg phosphorylation dynamics in live cells

Hoyoung Jung, Jung-Min Kee*

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

Protein Arg phosphorylation is a crucial post-translational modification (PTM) for stress response, virulence, and protein quality control of Gram-positive bacteria. Although this PTM was first discovered in the 1970s, it is only recently that a protein Arg kinase (McsB) and a pArg phosphatase (YwlE) have been identified in Gram-positive bacteria. McsB marks misfolded protein by Arg phosphorylation, and the pArg tag is recognized by the bacterial proteasome for degradation, analogous to protein ubiquitination in eukaryotes. Recently, we reported a CHEF-based fluorescent probe for real-time monitoring of Arg kinase/phosphatase activities *in vitro*. However, the peptide-based probe was not applicable to live-cell studies. To overcome this limitation, we developed new genetically encoded FRET-based enzyme activity probes for studying Arg phosphorylation dynamics in live cells. This sensor should be invaluable in studying the regulatory mechanisms of Arg phosphorylation dynamics.

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

Oral Presentations by Young Life Chemists

Room 105 THU 09:24

Chair: Woon Ju Song (Seoul National University)

Evolution of De Novo Designed Metal-dependent Glycosidases

WooJae Jeong, Woon Ju Song[1,*]

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

Metallo-hydrolases are ubiquitous in nearly all subclasses of hydrolases, utilizing metal elements to activate a water molecule and facilitate its subsequent association into diverse chemical bonds in substrates. However, metal-dependent glycosidase is unprecedented to date. Herein, we have designed non-canonical metal-dependent glycosidases by installing a coordinatively unsaturated and hydrolytically active zinc-binding site within a barrel-shaped outer membrane protein F (OmpF). Furthermore, we have evolved Zn-complexed OmpF variants by multiple rounds of screening. Our results present that the chemical power of metalloenzymes might provide the molecular basis for the discovery and development of novel metalloenzymes.

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

Oral Presentations by Young Life Chemists

Room 105 THU 09:36

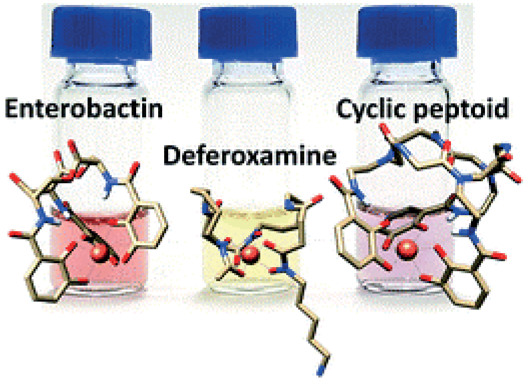
Chair: Woon Ju Song (Seoul National University)

Tris(catecholato) iron(III) complex formation with a nature-inspired cyclic peptoid ligand

Jinyoung Oh, Jiwon Seo[1,*]

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

Catechol is widely-known metal binding moieties used in natural metallophores. Researchers in various fields have investigated metal chelating abilities of catechol. Especially, enterobactin, which is one of catecholate siderophores, has received attention as a powerful metal-binding compound in nature. Herein, siderophore-mimicking macrocyclic peptoids were synthesized. Peptoid **3** with intramolecular hydrogen bonds showed an optimally arranged primary coordination sphere leading to a stable catecholate-iron complex. The tris(catecholato) structure of **3**-Fe(III) was determined with UV-vis, fluorescence, and EPR spectroscopies and DFT calculations. The iron binding affinity was comparable to that of deferoxamine, with enhanced stability upon air exposure. An increased ring size compared to that of enterobactin led to decreased iron affinity; however, the three extra residues left room for further chemical diversification or conjugation with other bioactive molecules. Our peptoid-Fe(III) complex may expand the field of siderophore mimicry toward novel sideromycin design or antibiotic strategies by nutritional immunity.



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

Oral Presentations by Young Life Chemists

Room 105 THU 09:48

Chair: Woon Ju Song (Seoul National University)

Understanding the substrate recognition of the peptide macrocyclase PsnB by structural and biochemical studies

Inseok Song, **Seokhee Kim**[1,*]

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

Ribosomally synthesized and post-translationally modified peptides (RiPPs) are a peptide based natural products that are ribosomally produced and undergo diverse post transcriptional modifications. Graspetides, a family of RiPPs, are multi-cyclic peptides that contain macrolactone or macrolactam linkages between their side-chain. Here, we discovered the molecular mechanism underlying substrate recognition of the PsnB, a macrocyclase that mediates the biosynthesis of plesiocin, a group 2 graspetide. Unlike other RiPPs, the core region of the precursor peptide exhibits high affinity to the PsnB through the conserved glutamate residues. This unusual enzyme-core interaction is even enhanced when leader peptide or nucleotide binds to the PsnB. We obtained complex structures of PsnB bound with its precursor and the nucleotide, and identified that the highly conserved Arg 213 of the PsnB specifically recognizes a ring-forming glutamate residue of core region of its precursor prior to phosphorylation. Structural analysis also revealed the conformational change of PsnB during the substrate binding. Binding of leader and nucleotide induces the conformational change of PsnB that provides proper core binding site. Collectively, We used biochemical studies and structural analyses to reveal the graspetide biosynthetic process, and provides insights into the molecular mechanism underlying substrate recognition in biosynthesis of graspetide.

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

Oral Presentation for Young Scholars in Organic Division

Room 201 THU 09:00

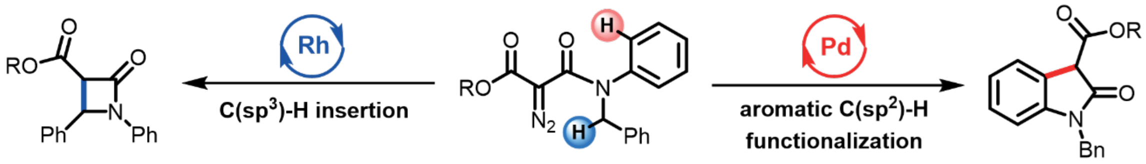
Chair: Han Yong Bae (Sungkyunkwan University)

Catalyst-Controlled Divergent C(sp^3)—H/C(sp^2)—H Bond Functionalization of Diazo Compounds

Yu lim Lee, Kyuin Choi, Sang-gi Lee*

Chemistry and Nanoscience, Ewha Womans University, Korea

Transition-metal catalyzed C—H bond functionalization induced by carbene, which is derived from the decomposition of diazo compound, is one of the most efficient and reliable synthetic tools for the formation of C—C bonds. Especially, controlling the regioselectivity over the site of functionalization is highly challenging yet important goal, wherein it could control the reaction pathway to provide the access for structurally different products from the same reactant. Herein, we present an unprecedented example of catalyst-controlled divergent functionalizations of C(sp^3)—H/C(sp^2)—H bonds of *N*-alkyl-*N*-aryl diazo amides. In the presence of rhodium catalyst, the diazo compounds undergo C(sp^3)—H bond insertion furnishing β-lactams, whereas the electrophilic aromatic C(sp^2)—H bond functionalization was occurred in the presence of palladium catalyst to afford indolin-2-one derivatives. Moreover, it was found that the selectivity was largely be determined by the presence of ester group in diazo amides. DFT calculation provided an insight on the role of ester functionality in such selectivity.



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

Oral Presentation for Young Scholars in Organic Division

Room 201 THU 09:12

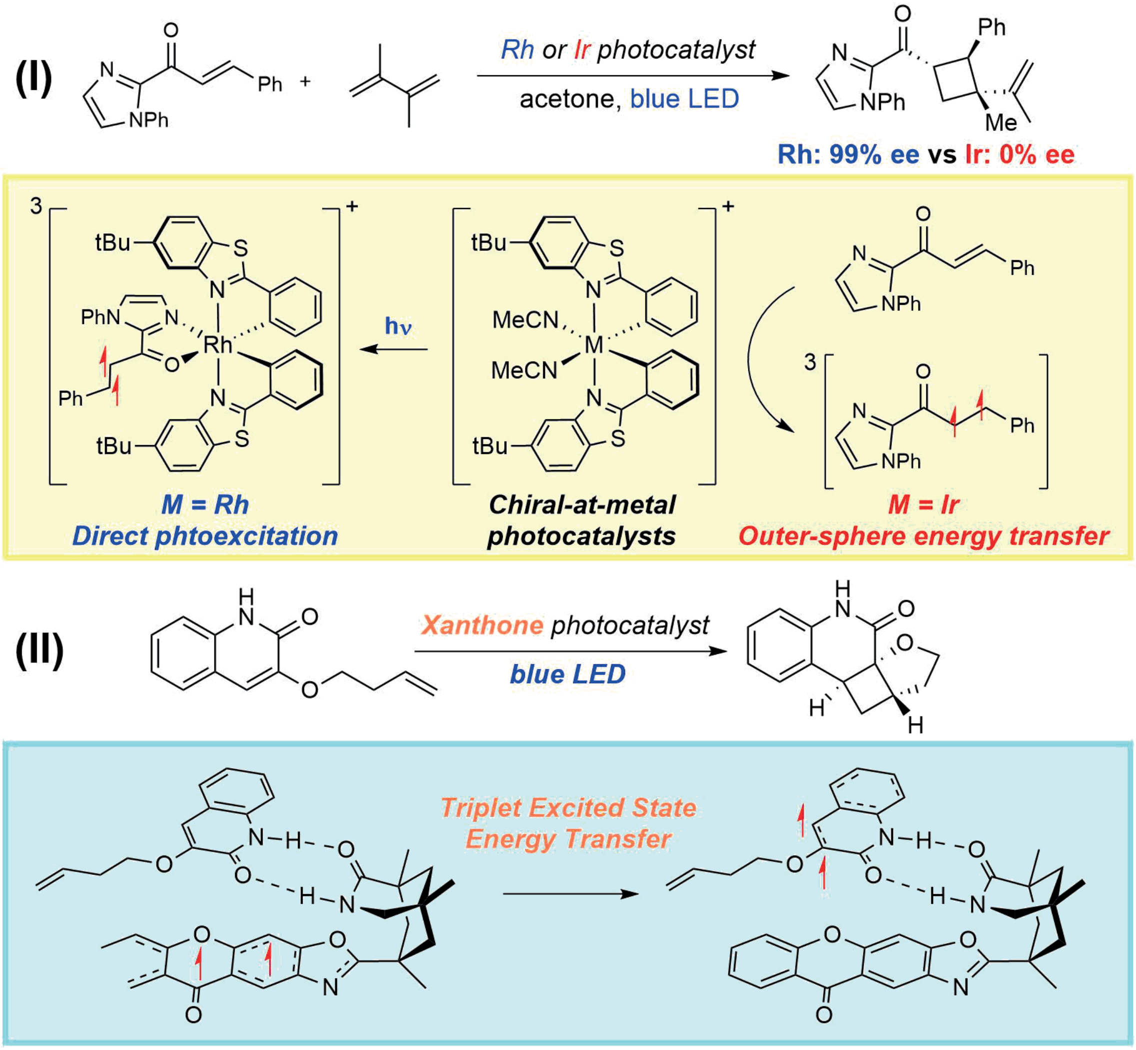
Chair: Han Yong Bae (Sungkyunkwan University)

Understanding the mechanisms of photo-activated [2 + 2] cycloadditions mediated by chiral organic and transition-metal photocatalysts

Jiyong Park[*], Hoimin Jung[1], Mu-Hyun Baik[2,*]

Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*
[2]*Chemistry, Korea Advanced Institute of Science and Technology, Korea*

In the last decade, chiral triplet sensitizers have emerged as powerful photocatalysts that can engender triplet excited-state intermediates. Upon light absorption, the catalysts access triplet excited-state electronic manifolds and activate desired substrates via the triplet-triplet energy transfer (TTEnT) known as the Dexter process. As the TTEnT occurs in the chiral constrict provided by the photocatalyst, the transformations can induce stereoenriched outcomes. However, the detailed mechanistic pathway toward the excited–state energy transfer, however, has not been explored in detail, impeding the rational design of chiral photocatalytic transformations based on TTEnT. Herein, we explored the mechanistic details of [2 + 2] cycloadditions catalyzed by bis-cyclometalated Rh/Ir complexes and chiral-xanthone photocatalysts, by means of the ground state and the excited state electronic structure methods. For the transition metal photocatalysis, we show that the Rh-based complex yields excellent enantioselectivity via the direct photoactivation mechanism, whereas the Ir results in racemates via the outer-sphere triplet energy transfer. For the chiral-xanthone catalyst, we demonstrate that the TTEnT is the rate-determining step of the entire catalytic cycle. Our computational analysis provides a detailed mechanistic understanding of the emerging class of catalytic transformations that will aid the further development of novel photocatalytic transformations.[1] Jung, H.; Hong, M.; Marchini, M.; Villa, M.; Steinlandt, P. S.; Huang, X.; Hemming, M.; Meggers, E.; Ceroni, P.; Park, J.; Baik, M.-H., Chem. Sci. 12, 9673-9681 (2021)


(I)
Rh or Ir photocatalyst
acetone, blue LED
Rh: 99% ee vs Ir: 0% ee
hν
M = Rh
Direct phtoexcitation
Chiral-at-metal
photocatalysts
M = Ir
Outer-sphere energy transfer
(II)
Xanthone photocatalyst
blue LED
Triplet Excited State
Energy Transfer

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

Oral Presentation for Young Scholars in Organic Division

Room 201 THU 09:24

Chair: Han Yong Bae (Sungkyunkwan University)

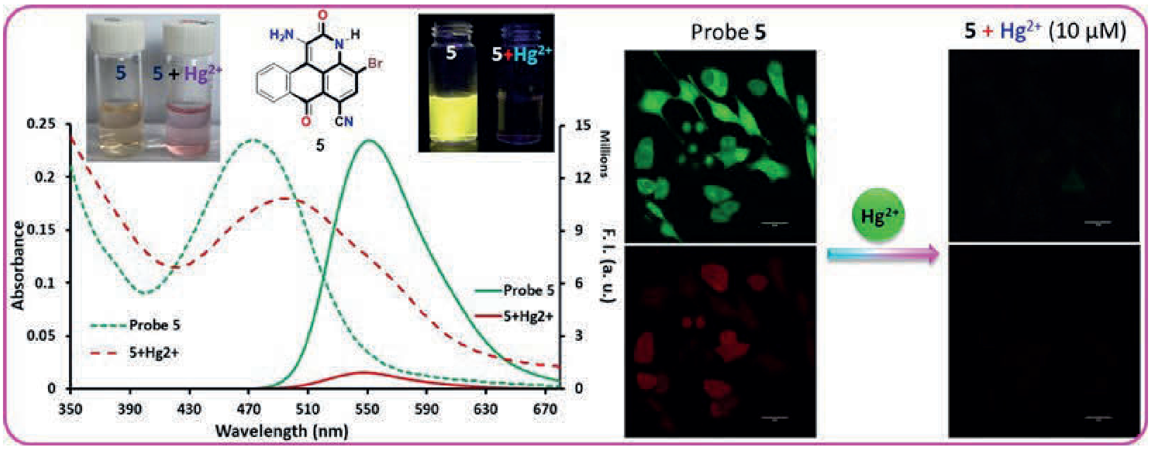
Naphthoquinolinedione-based probes with chromofluorogenic property for sensitive detection Hg^{2+} in aqueous solutions

Ashwani Kumar, **Pil Seok Chae**[1,*]

Department of Bio Nano, Hanyang University, India

[1]*Department of Bionano Engineering, Hanyang University, Korea*

AbstractMercury ion is an industrial and environmental toxin that needs to be monitored and regulated in aqueous samples.[1] We prepared six probes (**1**–**6**) using a naphthoquinolinedione ring as a platform for a fluorophore that contains different substituents on the quinolone ring. While all the probes investigated here showed the abilities to selectively bind Hg^{2+}, probe **5** with Br and CN substituents on the quinolone ring was most effective for the sensitive detection of Hg^{2+} in aqueous solutions. This probe showed a naked-eye color change from yellow to purple upon binding to Hg^{2+}. Fluorescence-based LODs of this probe were 5 nM (observed) and 0.047 pM (calculated). When bio-samples such as human urine and serum were used as media, the LOD of this probe for Hg^{2+} detection increased to 50 nM. Based on the results of DLS, FE-SEM, and DFT calculations, the quenching of probe fluorescence appears to be caused by large aggregates and photo-induced electron transfer (PET) upon Hg^{2+} binding. Probe **5** also showed the good ability to sense Hg^{2+} within human skin cancer cell (SK-MEL28). **References**1). T.W. Clarkson, L. Magos, Crit. Rev. Toxicol., 36 (2006) 609-662. 2). J. Li, D. Yim, W.-D. Jang, J. Yoon, Chem. Soc. Rev. 46 (2017) 2437-2458.3). A. Kumar, P.S. Chae, Sens. Actuator B 281 (2019) 933-944.


5
5 + Hg2+
H2N
O
N
H
Br
O
CN
5
5
5+Hg2+
Probe 5
5 + Hg2+ (10 μM)
Hg2+
0.25
0.2
0.15
0.1
0.05
0
Absorbance
350
390
430
470
510
550
590
630
670
Wavelength (nm)
15
12
9
6
3
0
Millions
F. I. (a. u.)
Probe 5
5+Hg2+
Probe 5
5+Hg2+

Oral Presentation : **ORGN.O-4**
Oral Presentation for Young Scholars in Organic Division
Room 201 THU 09:36
Chair: Han Yong Bae (Sungkyunkwan University)

Strategic Approach for Enhancing Sensitivity of Ammonia Gas Detection: Molecular Design Rule and Morphology Optimization for Stable Radical Anion Formation of Rylene Diimide Semiconductors

Byeong M. Oh, Jong Hyun Kim*

Department of Molecular Science and Technology, Ajou University, Korea

Herein, a strategic approach to enhance the sensitivity of ammonia gas detection using organic semiconductors by boosting the efficiency of ammonia gas-induced stable radical anion formation (SRAF) is reported. This is achieved through rational molecular design and engineering of field-effect transistors (FETs). New rylene diimide derivatives are designed and used to prepare molecular templates for efficient SRAF in thin films, and they are applied as gas-adsorbing active layers in FETs. Substituting linear-shaped perfluoroalkyl (PF) groups to π-electron-deficient naphthalene diimide (NDI) backbone enhances the ammonia gas detection limit to 200 ppb, attributed to the strong electron-withdrawing capability and low steric hindrance of PF groups. Replacing the core backbone (NDI) with perylene diimide (PDI) while retaining the PF group further enhances gas responsivity up to 18.17 (1700% increase in current) due to the enlarged π-conjugated bridge area. Computational characterization further supports that high electron affinity of the PDI-PF molecules and a larger gas-adsorption area in the PDI core result in the exceptional ammonia gas sensitivity. In addition, beneficial molecular orientation and nanopore formation of PDI-PF facilitate gas adsorption, resulting in remarkably enhanced gas-responsivity. The results indicate that molecular engineering for high-efficiency SRAF suggests a new strategy for developing high sensitivity ammonia sensing platforms.

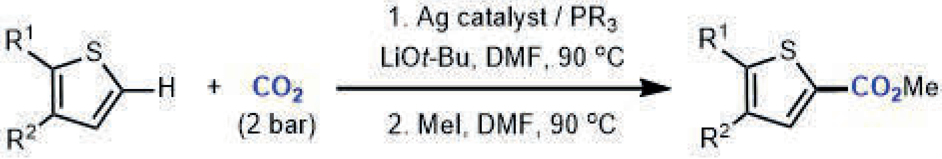
Oral Presentation : **ORGN.O-5**
Oral Presentation for Young Scholars in Organic Division
Room 201 THU 09:48
Chair: Han Yong Bae (Sungkyunkwan University)

Direct carboxylation of thiophene derivatives via Ag(I)-catalysis

Mijung Lee, Young Kyu Hwang*, Jaesung Kwak[1],*

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

Direct carboxylation of (hetero)aromatic compounds is particularly attractive because the corresponding carboxylic acids are ubiquitous structural motifs found in pharmaceuticals, organic materials, and commodity chemicals. [1] Numerous methods for synthesis of carboxylic acids have been developed, however direct carboxylation approach using CO_2 as C1 feedstock is more attractive method from an environmental perspective. [2] Due to the high thermodynamic stability of CO_2, most of the C–H carboxylation reactions proceed via a reactive carbanion intermediate, which is accessed by the use of high energy chemicals such as Grignard reagents or alkyl lithium reagents. However, these reactions generally require low reaction temperature and suffered from low functional group tolerance. [3] Herein, we report the first Ag(I)-catalyzed sp^2 C–H carboxylation of thiophene derivatives. [4] This catalytic system enables direct carboxylation of thiophene derivatives with a broad functional group tolerance under mild reaction conditions.Reference[1] Liu, Q.; Wu, L.; Jackstell, R.; Beller, M. Using carbon dioxide as a building block in organic synthesis. Nat. Commun. 2015, 6, 5933.[2] Banerjee, A.; Dick, G. R.; Yoshino, T.; Kanan, M. W. Carbon dioxide utilization via carbonate-promoted C–H carboxylation. Nature 2016, 531, 215. [3] Boogaerts, I. I. F.; Nolan, S. P. Carboxylation of C−H Bonds Using N-Heterocyclic Carbene Gold(I) Complexes. J. Am. Chem. Soc. 2010, 132, 8858–8859.[4] M, Lee.; Y, K, Hwang.; J, Kwak.; Ag(I)-Catalyzed C-H Carboxylation of Thiophene Derivatives. Organometallics Manuscript in revision.



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

Oral Presentation for Young Scholars in Organic Division

Room 201 THU 10:00

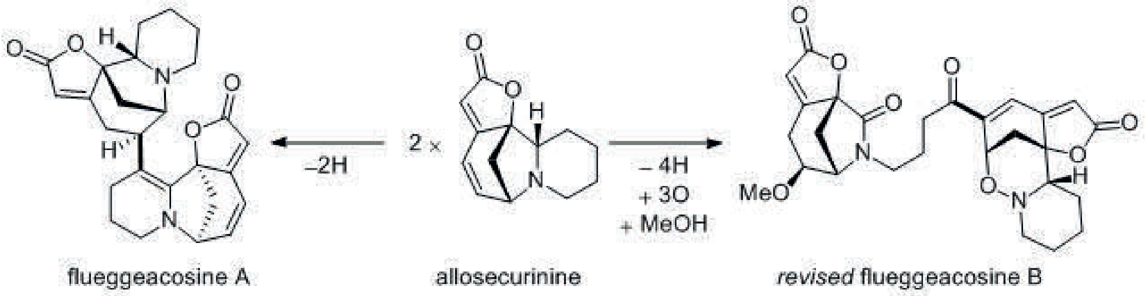
Chair: Han Yong Bae (Sungkyunkwan University)

Synthesis of dimeric high-oxidation state securinega alkaloids

Gyumin Kang, Sunkyu Han*

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

Presented here is the strategic evolution toward dimeric high-oxidation state securinega alkaloid flueggeacosine B[1] from allosecurinine. Three synthetic routes were developed aiming for improved atom-[2], step-economy[3] and ideality[4]. In the course of the strategic evolution, synthesis of flueggeacosine A and structure revision of flueggeacosine B were achieved. Eventually, flueggeacosine B could be accessed in 3 steps (LLS) from allosecurinine via a newly developed dehydrogenative cross-electrophile coupling reaction.**References**1. Wu, Z.-L.; Huang, X.-J.; Xu, M.-T.; Ma, X.; Li, L.; Shi, L.; Wang, W.-J.; Jiang, R.-W.; Ye, W.-C.; Wang, Y. *Org. Lett.* **2018**, *20*, 7703–7707.2. Trost, B. M. *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 259–281.3. Newhouse, T.; Baran, P. S.; Hoffmann, R. W. *Chem. Soc. Rev.* **2009**, *38*, 3010–3021.4. Gaich, T.; Baran, P. S. *J. Org. Chem.* **2010**, *75*, 4657–4673.



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

Oral Presentation for Young Scholars in Organic Division

Room 201 THU 10:12

Chair: Han Yong Bae (Sungkyunkwan University)

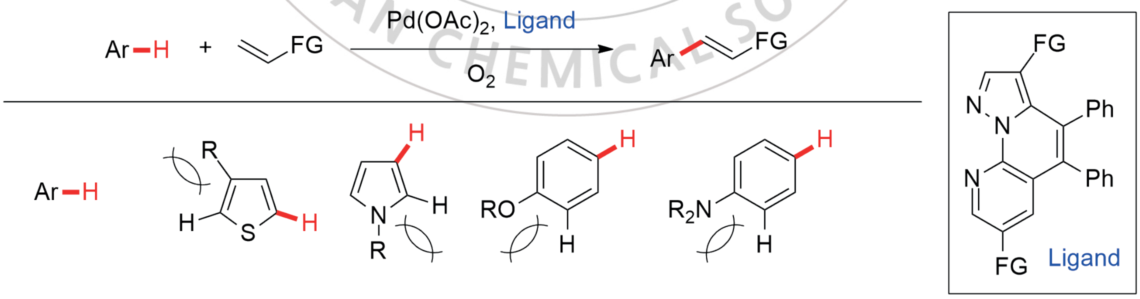
Ligand-Controlled Regioselective C–H Alkenylation at Sterically Unhindered Sites of (Hetero)arenes

Eunsu Kang, Jung Min Joo[1,*]

Department of chemistry, Pusan National University, Korea

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

A new class of ligands has been developed for direct C–H functionalization reactions. The use of tricyclic bidentate pyrazolonaphthyridine (PzNPy) ligands enabled regioselective alkenylation at sterically unhindered sites of (hetero)arenes. The installation of a pyrazole ring, which is less electron-rich than a pyridine ring, facilitated alkenylation reactions of electron-rich (hetero)arenes. In addition, rigid tricyclic PzNPy ligands promoted the reoxidation of Pd(0) species under oxygen, superior to bicyclic pyrazolopyridine (PzPy) ligands. Electronically tailorable PzNPy ligands improved efficiency of alkenylations of a wide range of (hetero)arenes.



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

Oral Presentation for Young Scholars in Organic Division

Room 201 THU 10:24

Chair: Han Yong Bae (Sungkyunkwan University)

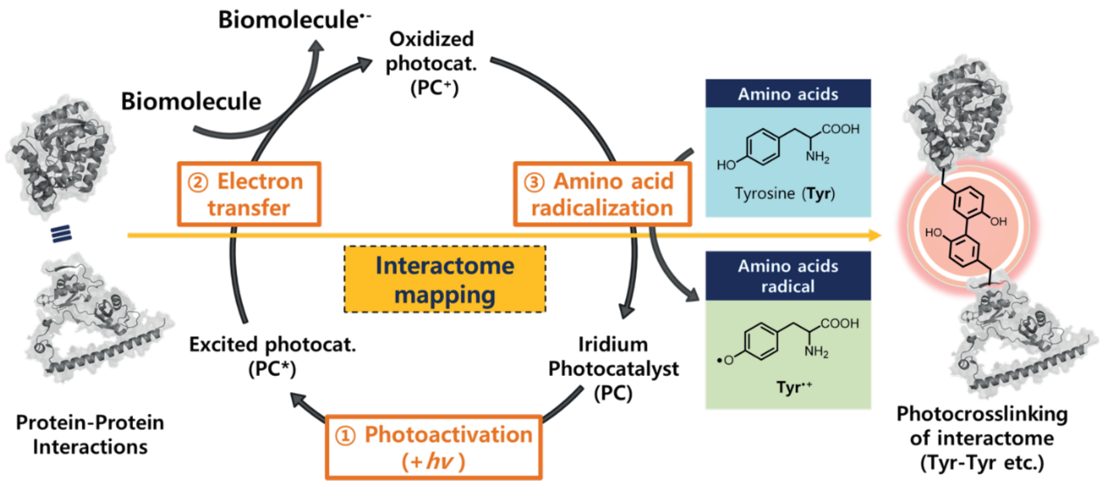
Spatially Resolved Interactome Mapping through Intracellular Protein-specific Photo-crosslinking in Live Cells

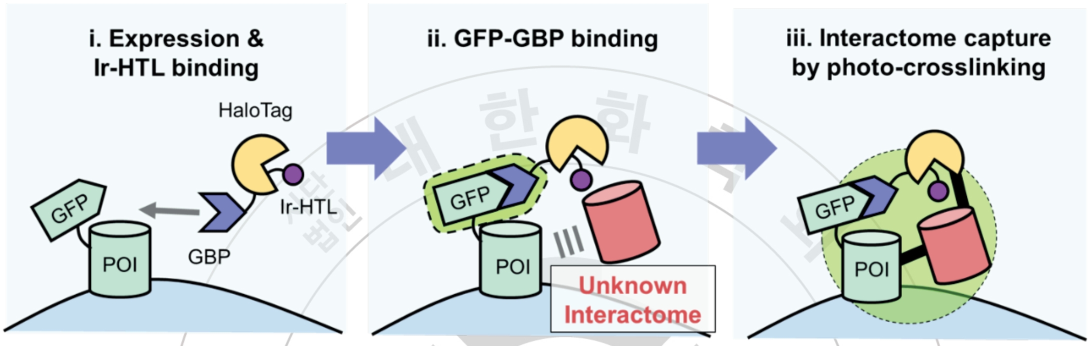
Jung Seung Nam, Hyun-Woo Rhee[1,*], Tae-Hyuk Kwon[*]

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

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

Direct photo-crosslinking reaction utilizing single photocatalyst has great value in exploring the protein-protein interactions (PPIs) because it results in direct coupling of nearby residues of surrounding interactome. Though photocatalytic crosslinking of proteins is accomplished to in vitro, its extension to living cell is a considerable challenge. Exploiting the worthwhile chemical reaction induced by photoactivation of organometallic iridium catalyst, we devise new method for mapping PPIs in living cells. Our method demonstrates applicability for intracellular regions with spatiotemporal resolution and following implementation to three different protein of interests. This advanced protein mapping method to utilize direct photo-crosslinking reaction can be expanded to various target proteins including even undruggable, and accelerate new discovery on underlying portion of the huge protein interaction network.


Biomolecule•⁻
Oxidized photocat. (PC⁺)
Biomolecule
② Electron transfer
③ Amino acid radicalization
Interactome mapping
Excited photocat. (PC*)
Iridium Photocatalyst (PC)
① Photoactivation (+hν)
Protein-Protein Interactions
Amino acids
COOH
NH₂
HO
Tyrosine (Tyr)
Amino acids radical
•O
Tyr•⁺
HO
OH
Photocrosslinking of interactome (Tyr-Tyr etc.)


i. Expression & Ir-HTL binding
HaloTag
GFP
POI
GBP
Ir-HTL
ii. GFP-GBP binding
GFP
POI
Unknown Interactome
iii. Interactome capture by photo-crosslinking
GFP
POI

Oral Presentation : **ORGN.O-9**
Oral Presentation for Young Scholars in Organic Division
Room 201 THU 10:36
Chair: Han Yong Bae (Sungkyunkwan University)

Water-Driven Biomimetic Catalytic Enantioselective Protonation: Physical Origin of On-Water Effect

Si Joon Park, Choong eui Song*

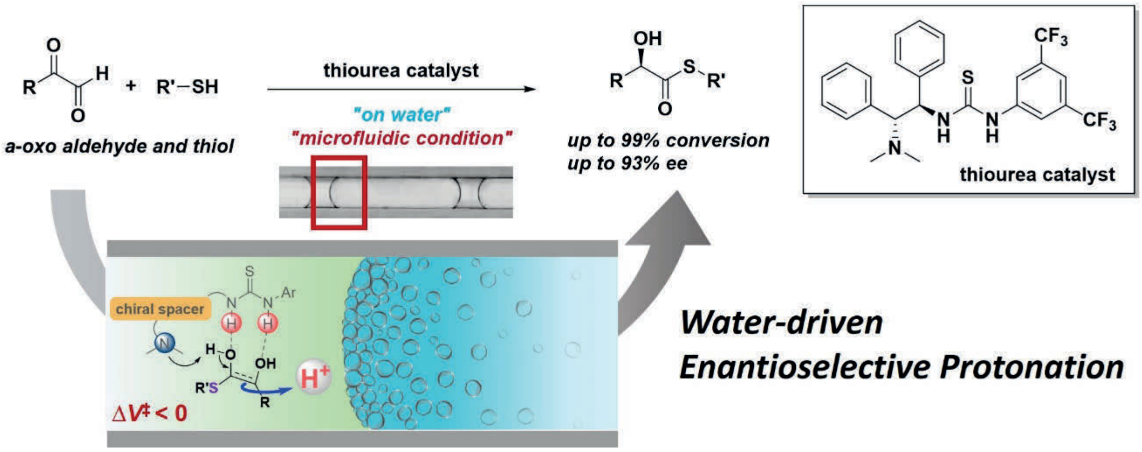
Department of Chemistry, Sungkyunkwan University, Korea

Catalytic enantioselective protonation of a prochiral carbanion in water is a common transformation in biological systems, but has been beyond the capability of synthetic chemists since unusually rapid movement (1−2 ps) of a proton in water leads to uncontrolled racemic protonation. Therefore, governing the movement of a proton in water within a catalytic cycle in an enantioselective manner is an extremely challenging task. In this symposium, we present a successful example of bio-inspired enantioselective protonation in water, revealing how to govern the movement of a highly mobile proton in water in an enantioselective manner.[1]Water enables a highly enantioselective glyoxalase I-mimic catalytic isomerization[2] of hemithioacetals which proceeds via enantioselective protonation of an ene-diol intermediate. The use of on-water condition turns on this otherwise extremely unreactive catalytic reaction as a result of the strengthened hydrogen bonds of water molecules near the hydrophobic reaction mixture. Furthermore, under on-water conditions, especially under biphasic microfluidic on-water conditions, access of bulk water into the enantio-determining transition state is efficiently blocked, consequently enabling the enantioselective introduction of a highly ungovernable proton to a transient enediol intermediate, which mimics the action of enzymes.

References

[1] Park, S.-J.; Hwang, I.-S.; Chang, Y. J.; Song, C. E. *J. Am. Chem. Soc.* **2021**, *143*, 2552−2557.

[2] Park, S. Y.; Hwang, I. S.; Lee, H. J.; Song, C. E. *Nat. Commun.* **2017**, *8*, 14877.



Water-driven Enantioselective Protonation

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

Oral Presentation for Young Scholars in Organic Division

Room 201 THU 10:48

Chair: Han Yong Bae (Sungkyunkwan University)

Scyllo-inositol-derived amphiphilic saccharides for membrane protein study

Aiman Sadaf, Pil Seok Chae[1,*]

Department of Bio-Nano Engineering, Hanyang University, Pakistan

[1]*Department of Bionano Engineering, Hanyang University, Korea*

Detergents are indispensable tools for keeping membrane proteins stable in aqueous media. Detergent stabilization efficacy is the direct manifestation of its molecular design. Classical detergents due to their limited structural diversity are of limited utility. Therefore, development of new detergents with distinct structures is necessary for membrane protein structural study. In this presentation, we introduce rigid core-bearing glycosides derived from scyllo-inositol (SIGs). The new detergent can be categorized into three different sets depending on the precise structure of the head groups: trimaltosides (STMs), ethylene glycol-conjugated trimaltosides (STM-Es) and hexa-glucosides (SHGs). When tested with a set of model membrane proteins, several SIGs were superior to the gold standard detergent DDM. Among the tested SIGs, STM-12 was most notable in preserving the stability of the multiple membrane proteins. The comparative study of three classes of SIGs enabled us to make the correlation of alkyl chain length and head group architecture with detergent efficacy for protein stabilization, thereby contributing to the expansion of detergent design tool-kit.

Oral Presentation : **MEDI.O-1**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 09:10
Chair: Sang Min Lim (KIST)

Identification of thieno[3,2-d]pyrimidine derivatives as dual inhibitors of focal adhesion kinase and FMS-like tyrosine kinase 3

Injae Shin, Taebo Sim*

Severance Biomedical Science Institute, Yonsei University College of Medicine, Korea

Focal adhesion kinase (FAK) is over-expressed in highly invasive and metastatic cancers. In order to identify novel FAK inhibitors, we designed and synthesized various thieno[3,2-d]pyrimidine derivatives. An intensive SAR study led to the identification of compound 26 as a lead. Moreover, compound 26, a multi-targeted kinase inhibitor, possesses excellent potencies against FLT3 mutants as well as FAK. Gratifyingly, compound 26 remarkably inhibits recalcitrant FLT3 mutants including F691L that cause drug resistance. Importantly, compound 26 is superior to PF-562271 in terms of apoptosis induction, anchorage-independent growth inhibition and tumor burden reduction in MDA-MB-231 xenograft mouse model. Also, compound 26 causes regression of tumor growth in MV4-11 xenograft mouse model, indicating that it could be effective against acute myeloid leukemia (AML). Finally, in an orthotopic mouse model using MDA-MB-231, compound 26 remarkably prevents metastasis of orthotopic tumors to lymph nodes. Taken together, the results indicate that compound 26 possesses potential therapeutic value against highly invasive cancers and relapsed AML.

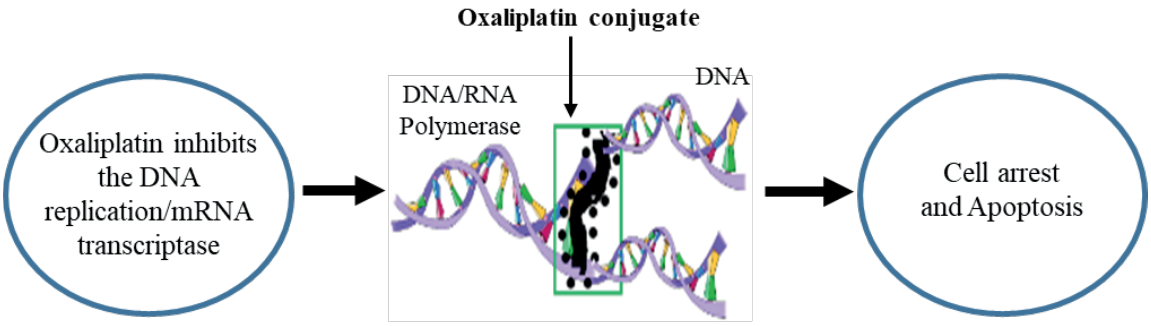
Oral Presentation : **MEDI.O-2**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 09:20
Chair: Sang Min Lim (KIST)

Intracellular delivery of oxaliplatin conjugate *via* cell penetrating peptide for the treatment of colorectal carcinoma *in vitro* and *in vivo*

Tejinder Singh, **Jungkyun Im**[1,*]

Department of Electronic Materials and Devices Engineering, Soonchunhyang University, Korea
[1]*Soonchunhyang University, Korea*

Abstract: Pt-based drugs are one of the main active agents in colorectal cancer treatment. However, drug resistance and dose-dependent side effects are the main barriers that restrict their clinical applications. As an alternative approach to these issues, we designed and synthesized a cell penetrating peptide (CPP) octaarginine-oxaliplatin conjugate that quickly and successfully delivered oxaliplatin into colon cancer cells. The CPP octaarginine is a well-studied cationic peptide that can play a role as a drug delivery vector. In this work, an octaarginine CPP (RRRRRRRR) was conjugated with oxaliplatin via a specific heterobifunctional linker. The *in vitro* studies showed the conjugate had affinity toward mitochondria inside cells and the MTT assay confirmed that conjugate is active in low micromolar range against colon cancer cells, requiring much lower concentrations than the oxaliplatin alone to reach IC$_{50}$. More importantly, in the *in vivo* mouse study, the conjugate effectively inhibited tumor growth and showed considerably high antitumor activity, demonstrating the conjugate can perform well *in vivo*. This strategy may offer a new approach for designing oxaliplatin derivatives or prodrugs with remarkable therapeutic capabilities.**References:**1.Abramkin, S., Valiahdi, S.M., Jakupec, M.A., Galanski, M., Metzler-Nolte, N. and Keppler, B.K., 2012. Solid-phase synthesis of oxaliplatin–TAT peptide bioconjugates. Dalton Transactions, 41(10), pp.3001-3005.2.Singh, T., Murthy, A.S., Yang, H.J. and Im, J., 2018. Versatility of cell-penetrating peptides for intracellular delivery of siRNA. Drug delivery, 25(1), pp.1996-2006.3.Singh, T., Kang, D.H., Kim, T.W., Kong, H.J., Ryu, J.S., Jeon, S., Ahn, T.S., Jeong, D., Baek, M.J. and Im, J., 2021. Intracellular Delivery of Oxaliplatin Conjugate via Cell Penetrating Peptide for the Treatment of Colorectal Carcinoma in vitro and in vivo. International Journal of Pharmaceutics, p.120904.4.Scheeff, E.D., Briggs, J.M. and Howell, S.B., 1999. Molecular modeling of the intrastrand guanine-guanine DNA adducts produced by cisplatin and oxaliplatin. Molecular Pharmacology, 56(3), pp.633-643.



Mechanism of Action of Oxaliplatin

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

Oral Presentation of Young Medicinal Chemists

Room 106 FRI 09:30

Chair: Sang Min Lim (KIST)

Peripheral Selective Oxadiazolylphenyl Alanine Derivatives as Tryptophan Hydroxylase 1 Inhibitors for Obesity and Fatty Liver Disease

Eunjung Bae, Jin hee Ahn*

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

Tryptophan hydroxylase 1 (TPH1) has been recently suggested as a promising therapeutic target for treating obesity and fatty liver disease. A new series of 1,2,4-oxadiazolylphenyl alanine derivatives were identified as TPH1 inhibitors. Among them, compound 23a was the most active in vitro, with an IC50 (half-maximal inhibitory concentration) value of 42 nM, showed good liver microsomal stability, and showed no significant inhibition of CYP and hERG. Compound 23a inhibited TPH1 in the peripheral tissue with limited BBB penetration. In high-fat diet-fed mice, 23a reduced body weight gain, body fat, and hepatic lipid accumulation. Also, 23a improved glucose intolerance and energy expenditure. Taken together, compound 23a shows promise as a therapeutic agent for the treatment of obesity and fatty liver diseases.

Oral Presentation : **MEDI.O-4**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 09:40
Chair: Sang Min Lim (KIST)

Enantioselective Total Synthesis of (-)-Verrucarol for the Development of Anticancer Drug Against Triple-Negative Breast Cancer

Sang Jeon Chung*, Eun Seok Choi[1], Wonyoung Jang[1], Seung Bin Park[1]

College of Pharmacy, SungKyunKwan University, Korea
[1]*College of Pharmacy, Sungkyunkwan University, Korea*

Triple-negative breast cancer (TNBC) is the most aggressive subtype of breast cancer. Therefore, there is no effective therapeutic option and the development of new therapeutic strategies for the treatment of TNBC has become an urgent medical need. Type D trichothecene mycotoxin are highly potent and for development of anti-breast cancer drugs. A common structure feature of type D trichothecene mycotoxin is the verrucarol. Verrucarol based macrocyclic trichothecene are known as promising anticancer therapeutic candidate.Here, we have developed an enantioselective total synthesis of a type D trichothecene verrucarol. The route is based on a retrosynthetic strategy that was devised to facilitate the synthesis of key core bicyclic lactone which enabled efficient and concise total synthesis. A highly enantioselective catalysis sets the quaternary stereocenter by the catalytic asymmetric alkylation of β-keto esters. Phase transfer N-spiro C_2-symmetric chiral quaternary ammonium salt (S,S-1) catalyst was used to facilitate the direct stereo controlled formation of quaternary stereocenter which formed the structural skeleton of trichothecene with desired stereochemistry. The subsequent reaction sequences were lactonization, aldol reaction, Dieckmann condensation and Barton-Crich's decarboxylative oxygenation resulting in a 6,5,5 ring system. Then the ring expansion took place to form a keto group at the methylene bridge between ring B and C. At the later stage epoxidation was achieved to form verrucarol. We present a synthesis which is effective, robust, and reproducible at large scale.

Oral Presentation : **MEDI.O-5**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 09:50
Chair: Sang Min Lim (KIST)

Discovery of Novel Sphingosine-1-Phosphate-1 ($S1P_1$) Receptor Agonists for the Treatment of Multiple Sclerosis

Sun Jun Park, Ki Duk Park[1,*]

Convergence Research Center for Dementia, Division of Bio-Med Science & Technology, Korea Institute of Science and Technology, KIST School, UST, Korea
[1] *Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

The sphingosine-1-phosphate-1 ($S1P_1$) receptor agonists have great potential to treat multiple sclerosis (MS) because they can inhibit lymphocyte egress through receptor internalization. We designed and synthesized azetidine, pyrrolidine and piperidine derivatives to discover a novel $S1P_1$ agonist for MS treatment. azetidine derivatives were determined to have excellent in vitro efficacy and drug-like properties. Among them, compound **21l** was found to have superior drug-like properties as well as excellent in vitro efficacies (EC_{50} = 7.03 nM in β-arrestin recruitment; EC_{50} = 11.8 nM in internalization). We also confirmed that **21l** effectively inhibited lymphocyte egress in the peripheral lymphocyte count (PLC) test and significantly improved the clinical score in the experimental autoimmune encephalitis (EAE) MS mouse model.

Oral Presentation : **MEDI.O-6**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 10:00
Chair: Sang Min Lim (KIST)

Heterobivalent ligands targeting both PSMA and hepsin for prostate cancer diagnosis.

Hyunsoo Ha, Youngjoo Byun[1,*]

Department of Pharmacy, Korea University Sejong Campus, Korea
[1]*Department of Pharmacy, Korea University, Korea*

Prostate cancer is one of the most common types of cancer in men. According to the National Cancer Center, the incidence of prostate cancer in Korea was 14,857 cases in 2018, which is 11.5% of the total. As the Korean lifestyle becomes more and more western, this upward trend is expected to continue. The 5-year survival rate for localized prostate cancer is quite high, close to 100%. However, the survival rate for metastatic cancer is 44.9%. Therefore, there is an urgent need to make an accurate diagnosis of prostate cancer at an early stage.Prostate-specific antigen (PSA) is widely used as a biomarker for prostate cancer in annual check-ups. However, the PSA test is not specific for prostate cancer because its level is elevated in benign prostate hyperplasia. New tools are needed for more accurate diagnosis of metastatic prostate cancer. Prostate-specific membrane antigen (PSMA), also called folate hydrolase or carboxypeptidase II, is an excellent biomarker for metastatic prostate cancer because it is highly overexpressed in metastatic prostate cancer. Hepsin is also an attractive biomarker because of its high expression in prostate cancer. Since PSMA and hepsin are a type II transmembrane protein and their enzymatic active sites are in the extracellular region, these proteins are considered as valuable targets for prostate cancer imaging. To identify new imaging agents for prostate cancer, we developed heterobivalent compounds that target both PSMA and hepsin. These compounds are expected to be more potent than those acting on a single target. We used an acetyl-Leu-Arg-ketothiazole (Ac-LR-kbt) as the hepsin-binding motif and a Lys-urea-Glu unit as the PSMA-binding motif. We introduced a PEG linker to modulate physicochemical properties and an optical dye (e.g., SulfoCy7 and SulfoCy3) for in vitro and in vivo imaging studies. The representative heterobivalent compound showed strong inhibition of both PSMA and hepsin protein at in vitro studies, suggesting that it may be developed as a new dual imaging probe for the diagnosis of prostate cancer.

Oral Presentation : **MEDI.O-7**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 10:10
Chair: Sang Min Lim (KIST)

Allosteric Inhibitors of Kidney Type Glutaminase for the Treatment of KEAP/NRF2 Genes Mutated Solid Tumors.

Krishna babu Duggirala, Kwangho Lee[1,*]

Medicinal Chemistry and Pharmacology, KRICT, India
[1]*Korea Research Institute of Chemical Technology, Korea*

Glutamine is the most abundant amino acid in the blood. Glutaminase (GLS-1/2) catalyzes the hydrolysis of glutamine into glutamate and ammonia in mitochondria through glutaminolysis. Warburg effect explains glutaminolysis is the main energy source for the growth and viability of malignant tumors. GLS-1 was found to be overexpressed in many glutamine dependent cancer cells. Recent studies has disclosed that GLS-1 inhibition causes regression in the certain tumors categorized by mutation in Kelch-like ECH-associated protein (KEAP) and/or NRF2 genes, which encode for proteins that regulate glutathione production. Therefore, GLS has become a key target for small molecule therapeutic intervention. Numerous competitive inhibitors (DON) and allosteric inhibitors (like BEPTS, CB-839, etc.) were developed. However to date; CB-839 and IACS-6274 have entered clinical trials for the treatment of advanced solid tumors and hematological malignancies. Although several potent inhibitors have been developed, still drug-like properties were not optimum, there's a room to improve their potency and drug-like properties. We started, GLS-1 inhibitor discovery program focused on optimizing physicochemical and pharmacokinetic properties, and have developed a new selective inhibitor TRG-039, which exhibits similar potency to CB-839. Studies of drug-like properties ongoing results will published in near future.

Oral Presentation : **MEDI.O-8**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 10:20
Chair: Sang Min Lim (KIST)

Design and Synthesis of Unique Peptoid-Based Structures

Soomin Kim, Yong-Uk Kwon[*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

In order to explore the functional roles of each protein in biological systems, the development of structurally diverse chemical tools with a high affinity and a high specificity against proteins should be highly desired. Peptoids are structural isomers of peptides with the alkyl substitution appended to the amide nitrogen instead of the α-carbon of peptides. The absence of amide hydrogen in the backbone structure results in highly diverse structural and functional features, including proteolytic resistance and improved cell permeability. Additionally, structurally rigid cyclic peptoids have been in the spotlight for their enhanced proteolytic resistance and improved binding affinity against target proteins. Moreover, unique peptoid-based structures should be fascinating molecules in terms of challenging synthesis and promising potentials as molecular probes or chemical tools in the field of chemical biology, molecular recognition, etc.In this presentation, our efforts for the design and synthesis of interesting peptoid-based chemical tools by employing various orthogonal ligation reactions will be introduced. We first envisioned to create bridged peptoids via macrolactamization followed by ring-closing metathesis (RCM) and then designed sandwich-type peptoids with capping moiety via macrolactamization followed by a click reaction. Additionally, sphere-type peptoids were also constructed through a combination of chemically orthogonal macrocyclization strategies, namely, macrolactamization, disulfide bond formation, and RCM in quite high conversion yields. These results reveal the possibility for the development and application of various unique peptoid structures as molecular probes, transporters, or sensors in the field of chemical biology and drug discovery.

Oral Presentation : **MEDI.O-9**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 10:30
Chair: Sang Min Lim (KIST)

Design, Synthesis, and Biological Evaluation of New Peripheral 5HT2A Antagonists for Nonalcoholic Fatty Liver Disease

Minhee Kim, Jin hee Ahn[1,*]

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

Nonalcoholic fatty liver disease (NAFLD) is increasingly prevalent worldwide, causing serious liver complications, including nonalcoholic steatohepatitis (NASH). Recent findings suggest that peripheral serotonin (5-hydroxytryptamine, 5HT) regulates energy homeostasis, including hepatic lipid metabolism. More specifically, liver-specific 5HT2A knockout mice exhibit alleviated hepatic lipid accumulation and hepatic steatosis. Here, structural modifications of pimavanserin, a 5HT2A antagonist approved for the treatment of Parkinson's disease (CNS drug), led us to synthesize new peripherally acting 5HT2A antagonists. Among the synthesized compounds, compound 14a showed good in vitro activity, good liver microsomal stability, 5HT subtype selectivity, and no significant inhibition of CYP and hERG. The in vitro and in vivo Blood-Brain-Barrier permeability study proved that 14a acts peripherally. Compound 14a decreased the liver weight and hepatic lipid accumulation in high-fat diet-induced obesity mice. Our study suggests new therapeutic possibilities for peripheral 5HT2A antagonists in NAFLD.

Oral Presentation : **MEDI.O-10**
Oral Presentation of Young Medicinal Chemists
Room 106 FRI 10:40
Chair: Sang Min Lim (KIST)

Design and characterization of cereblon-mediated androgen receptor proteolysis-targeting chimeras

Akshay Takwale, Jong Yeon Hwang[1,*]

Medicinal chemistry and pharmacology, University of Science & Technology, India
[1]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

Proteolysis-targeting chimera (PROTAC)-mediated protein degradation is a rapidly emerging therapeutic intervention that induces the degradation of targeted proteins. Herein, we report the design and biological evaluation of a series of androgen receptor (AR) PROTAC degraders for the treatment of metastatic castration-resistant prostate cancer. Predominantly, instead of thalidomide, we utilized the TD-106 scaffold, a novel cereblon (CRBN) binder that was identified in our previous study. Our results suggest that the linker position in the TD-106 CRBN binder is critical for the efficiency of AR degradation. The compounds attached to the 6-position of TD-106 promoted better degradation of AR than those at the 5- and 7-positions. Among the synthesized AR PROTACs, the representative degrader 33c (TD-802) effectively induced AR protein degradation, with a degradation concentration 50% of 12.5 nM and a maximum degradation of 93% in LNCaP prostate cancer cells. Additionally, most AR PROTAC degraders, including TD-802, displayed good liver microsomal stability and in vivo pharmacokinetic properties. Finally, we showed that TD-802 effectively inhibited tumor growth in an in vivo xenograft study.

Oral Presentation : **MAT.O-1**
Oral Presentation for Young Material Chemists
Room 107 THU 09:00
Chair: Jaewon Lee (Chungnam National University)

An effective way of optimizing the photocatalyst functionality of semiconductor using co-hybridized conductive nanosheet

Namhee Kwon, Seong-Ju Hwang[*]

Department of Materials Science and Engineering, Yonsei University, Korea

For the exploration of high-performance visible-light-active photocatalyst, it is necessary to optimize several crucial factors of semiconductors such as light absorption region, lifetimes of photoexcited electron and hole, charge transport property, and photocatalysis kinetic. The hybridization with conductive species provides an efficient methodology to enhance the photocatalytic activity of semiconductor via the control of these factors. In this study, co-hybridized reduced graphene oxide (rGO) and RuO_2 nanosheets (NSs) are employed as effective conductive matrix for coupling with CdS photocatalyst. The electrostatically-derived self-assembly between cationic CdS quantum dots and homogeneously-mixed anionic RuO_2/rGO NSs yields strongly-coupled ternary nanohybrid with increased porosity. The ternary CdS-RuO_2/rGO nanohybrid exhibits notably higher photocatalytic activities than do binary CdS-RuO_2 or CdS-rGO homologues, underscoring the synergetic hybridization effect of flexible rGO and hydrophilic RuO_2 NSs. Of noteworthy is that co-hybridized NSs can play better roles of photosensitizers and cocatalysts than do single RuO_2 or rGO NSs, which is mainly responsible for remarkable improvement of photocatalytic activity upon the co-hybridization with mixed RuO_2/rGO NSs. The present study underlines that co-hybridization with complementary inorganic and graphene NSs can provide an efficient and economically-feasible methodology to explore novel high-performance catalyst materials.

Oral Presentation : **MAT.O-2**
Oral Presentation for Young Material Chemists
Room 107 THU 09:10
Chair: Jaewon Lee (Chungnam National University)

Molecular-level control of the intersheet distance and electronic coupling between 2D nanosheets to establish design rules for hybrid photocatalysts

Tae-Ha Gu, Seong-Ju Hwang[1,*]

Department of Chemistry and Nanoscience, Ewha Womans University, Korea
[1]*Department of Materials Science and Engineering, Yonsei University, Korea*

Hybridization with conductive nanospecies has attracted intense research interest as a general effective means to improve the photocatalytic functionalities of nanostructured materials. To establish universal design rules for high-performance hybrid photocatalysts, correlations between versatile roles of conductive species and interfacial interaction between hybridized species are systematically investigated through fine-control of intersheet distance between photocatalytically active TiO2 and metallic reduced graphene oxide (rGO) nanosheets. Molecular-level tailoring of intersheet distance and electronic coupling between 2D nanosheets can be successfully achieved by restacking of colloidal nanosheet mixture with variable-sized n-alkylamine molecules as intercalants. While the shortest intersheet distance between restacked TiO2 and rGO nanosheets leads to the highest visible-light-driven photocatalytic activity, the best UV-vis photocatalyst performance occurs for moderate intersheet spacing. These results highlight the greater sensitivity of photoinduced electronic excitation to the intersheet distance than that of interfacial charge transfer. The rGO nanosheet can function as effective charge transport pathway and cocatalyst within ~1.7 nm distance from the semiconducting nanosheet, and as efficient stabilizer for hybridized photocatalyst within ~1.8 nm. The present study underscores that the intercalative restacking of colloidal nanosheet mixture with intercalants enables molecular-level control of distance between 2D inorganic/graphene nanosheets, which provides a rational design strategy for high-performance hybrid photocatalysts.

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

Oral Presentation for Young Material Chemists

Room 107 THU 09:20

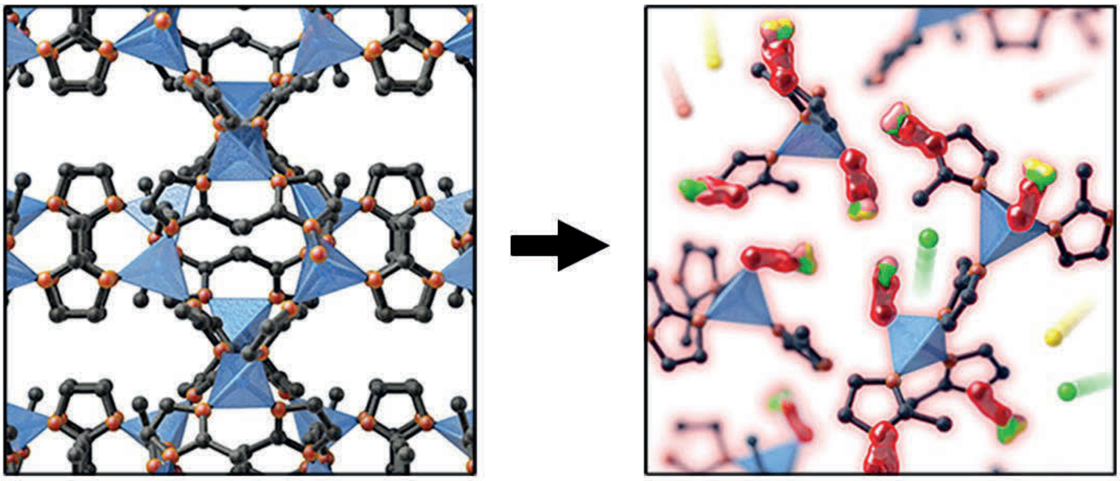
Chair: Jaewon Lee (Chungnam National University)

Highly affinitive metal-organic fragments torn from metal-organic frameworks for stabilizing catalysts

Won Ho Choi, Kyung Min Choi[1,*]

Institute of Advanced Materials and Systems, Sookmyung Women's University, Korea
[1]*Division of Chemical and Biomolecular Engineering, Sookmyung Women's University, Korea*

The development of support materials is one of the most critical challenges in a wide range of fields including energy, the environment, and catalysis. This is because support materials can endow guest materials with new properties. In catalysis, the catalyst–support interaction influences the catalytic performance, so it is urgently required to create a high-affinitive sites in porous supporting media. Among the promising candidate support materials, highly porous and crystalline metal–organic frameworks (MOFs) have received considerable attention. Although many MOFs have been successfully utilized as supports, their metal sites have a weak affinity for the guest material due to blockage by organic linkers. We hypothesized that the affinity could be increased by tearing the MOFs into smaller pieces based on this intrinsic limitation. Accordingly, in this work, we developed a new pathway for producing metal–organic fragments by tearing MOFs via hydrogen plasma bombardment. The hydrogen plasma exposed more metal nodes and created more delocalized electrons, resulting in high-affinity sites within the metal–organic fragments. As a result, the metal–organic fragments were successfully applied as highly affinitive support. The cobalt–imidazole fragments were thoroughly impregnated with tri-metallic FeNiMo, and the resulting electrocatalyst exhibited low overpotentials for oxygen evolution reaction. Moreover, the electrocatalyst showed strong durability for at least 45 days without loss of activity.



Metal-Organic Framework (MOF)

Metal-Organic Fragments with FeNiMo (CIF:FeNiMo)

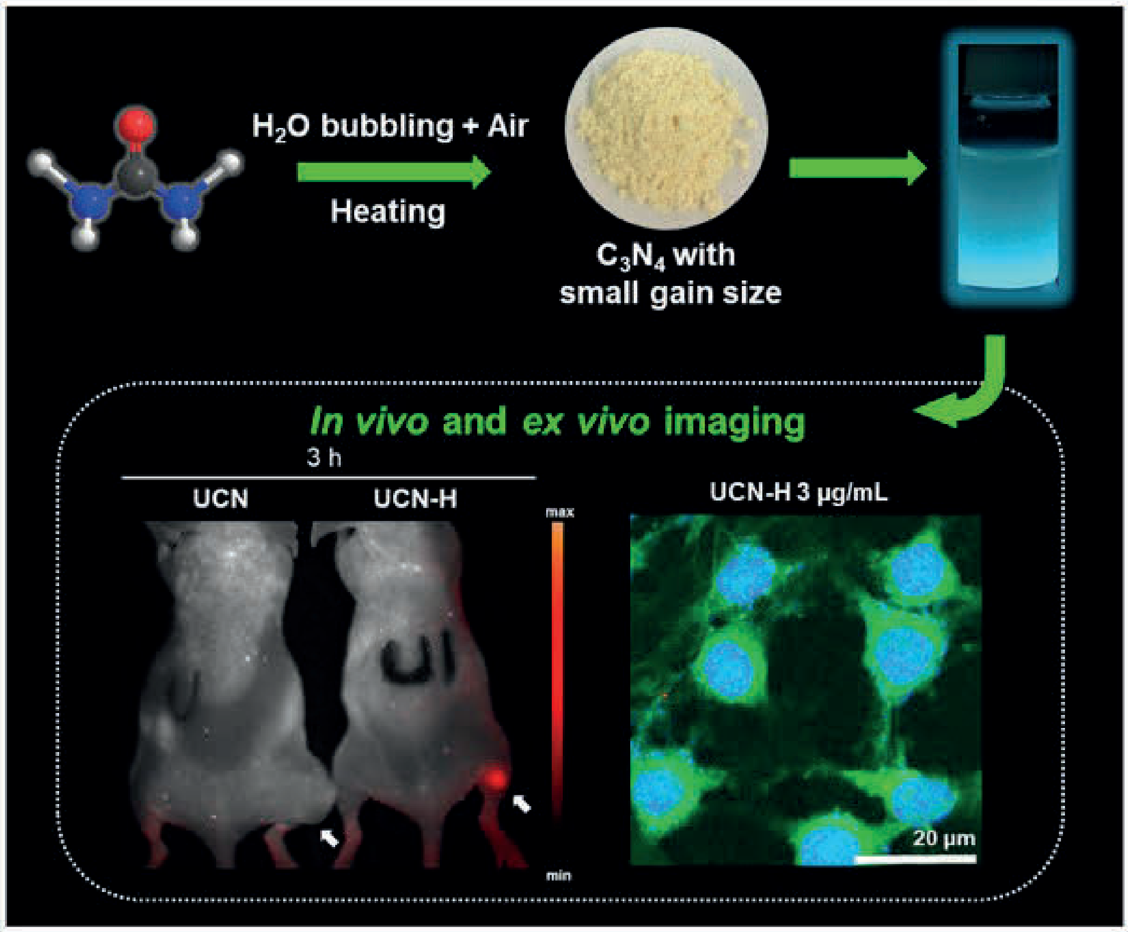
Oral Presentation : **MAT.O-4**
Oral Presentation for Young Material Chemists
Room 107 THU 09:30
Chair: Jaewon Lee (Chungnam National University)

Metal-free 2D C_3N_4-based nanoplatelets produced under humidified air gas for in vivo fluorescence imaging

Dawoon Jang, Sungjin Park*

Department of Chemistry, Inha University, Korea

In this work, we develop a route to produce a novel bioimaging probe framework. A C3N4 material (UCN-H) is produced by thermal condensation of urea under humidified air treatment. Chemical characterizations reveal that the UCN-H contains a C3N4 network with smaller grain sizes and more amine-based functionalities at the edges than UCN, which is separately produced with the humidified air treatment. 2D C3N4 nanoplatelets by generated sonication of the UCN-H powder, which highly stable aqueous dispersions including fluorescent. The photoluminescence (PL), time resolved-PL, and 2D excitation-emission spectra of the dispersions show that the UCN-H has less-intra bandgap traps and longer PL lifetime than UCN. In confocal microscopic study using the nanoplatelets, clear fluorescent cell-images are obtained without any cytosolic aggregation. In in vivo imaging studies with MDA-MB-231 tumor- bearing mice models, persistently strong fluorescence signals are successfully observed on tumor lesions without any interference of auto-fluorescence from live tissues after their accumulation by passive tumor targeting. Ex vivo biodistribution and histology results are well-matched with in vivo fluorescence imaging results.


H$_2$O bubbling + Air
Heating
C$_3$N$_4$ with
small gain size
In vivo and ex vivo imaging
3 h
UCN
UCN-H
max
min
UCN-H 3 µg/mL
20 µm

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

Oral Presentation for Young Material Chemists

Room 107 THU 09:40

Chair: Jaewon Lee (Chungnam National University)

Fabrication of Water-Repellent Platinum(II) Complex-Based Photon Downshifting Layers for Perovskite Solar Cells by Ultrasonic Spray Deposition

Eunhye Hwang, Chaiheon Lee, Sung-Yeon Jang[1,*], Kwanyong Seo[1,*], Tae-Hyuk Kwon[*]

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

[1]*School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*

Organic-inorganic hybrid perovskite solar cells (PSCs) have been regarded as one of the most promising photovoltaics due to the rapid growth of efficiency from 3.8% to 25.2%.[1] However, they exhibit relatively inefficient photocurrent generation in the UV region and severe degradation when exposed to UV light and humidity.

Herein, to enhance UV and humidity stability as well as photocurrent generating efficiency, a water-repellent platinum(II) complex, **Pt-F**, is developed as a luminescent photon downshifting layer (PDL) for PSCs. The **Pt-F** PDL is fabricated on the glass substrate of a PSC using ultrasonic spray deposition (USD), resulting in a considerably higher crystallinity and photoluminescence quantum yield (PLQY) than those fabricated by conventional spin-coating (PLQYs of 77% and 19%, respectively). A maximum device performance of 22.0% is achieved through the addition of a PDL coating to a 21.4% efficient PSC owing to the long-range photon downshifting effect of **Pt-F**, confirmed by the enhanced spectral response of the device in the UV region. Moreover, remarkable improvements in UV and humidity stability are observed in **Pt-F**-coated PSCs. The versatile effects of the **Pt-F**-based PDL, when fabricated by USD, suggest wide ranging applicability that can improve the performance and stability of other optoelectronic devices.[2]

References

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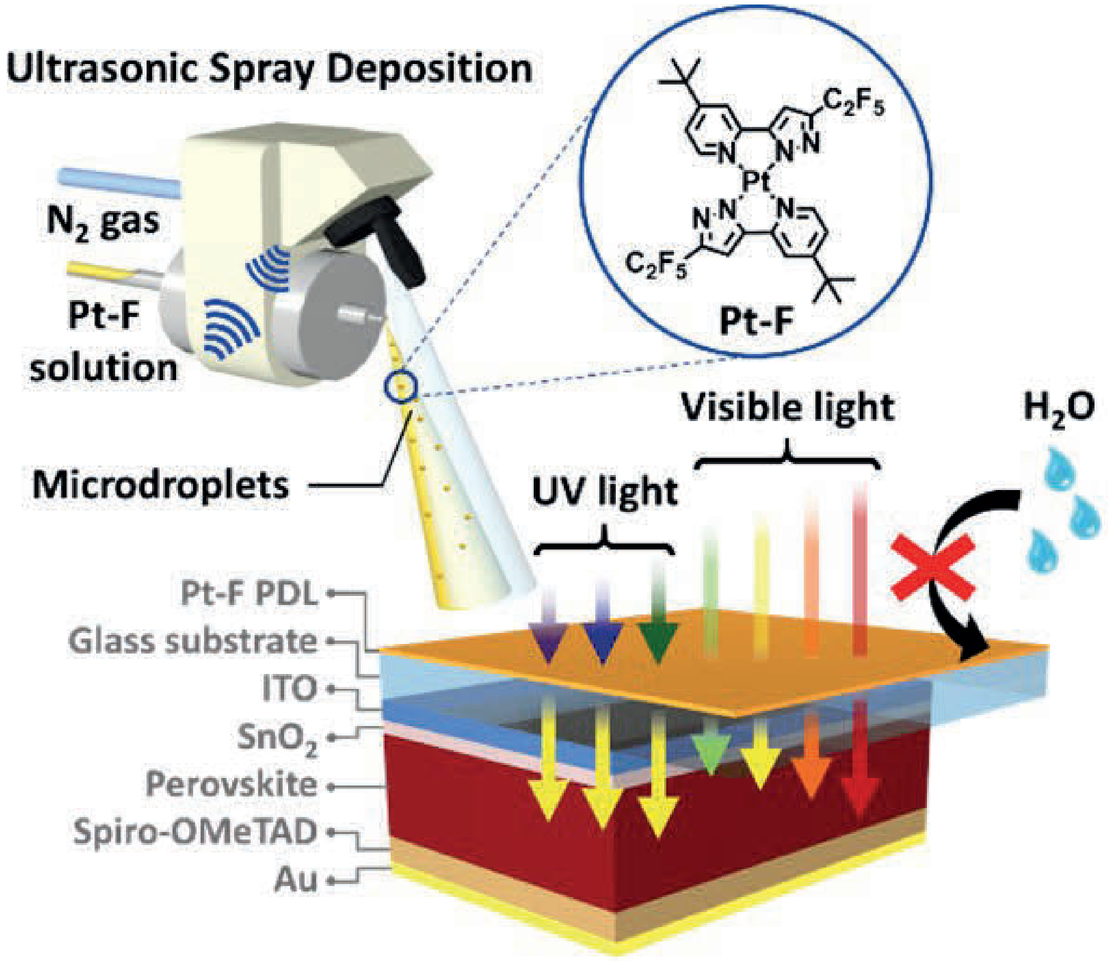
2. Hwang, E.; Kim, H.; Lee, S.-H.; Seo, J. H.; Kim, H.-T.; Lee, C.; Jang, S.-Y.; Seo, K.; Kwon, T.-H. *Adv. Energy Mater.* **2020**, 10, 2001238



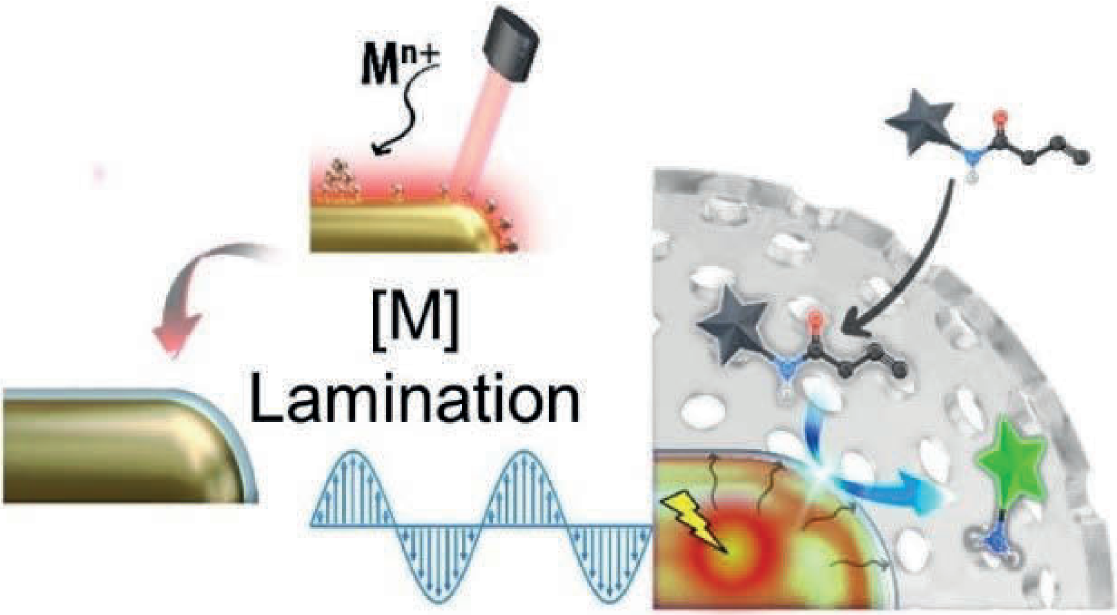
Oral Presentation : **MAT.O-6**
Oral Presentation for Young Material Chemists
Room 107 THU 09:50
Chair: Jaewon Lee (Chungnam National University)

Nanoreactors Carrying Atomically Conformal Metal Lamination on Plasmonic Nanocrystals for Efficient Catalysis

Anubhab Acharya, In Su Lee*

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

Development of a strategy endowing the impressive photocatalytic functionality in nanocrystals (NCs). Despite having a wide range of application potential in catalysis, electronics, displays, and magnetics, etc., the conformal deposition of noble transition metals (Pt, Pd, Ru, Rh) on plasmonic NCs (Au, Ag) to a critical limit of few-atomic-layer are scarce. We introduce “confine and shine” strategy to uniformly cover the distinct surface curvatures of plasmonic NCs with conformal ultrathin layers of various catalytic noble metals, similar to the process of lamination. Instead of any kinetic anisotropic metal deposition, the confined environment of hollow silica employs the platform to synthesize self-limited skinlike metal lamination by irradiating NIR laser to manipulate the atomic arrangement. The metal laminated plasmonic NCs preserve the hallmark plasmonic property of the core by avoiding severe non-radiative damping. Consequently, the plasmonic-catalytic hybrid nanoreactor can perform diverse photocatalytic transformations with magnificent rate.Reference : Acharya et al. J. Am. Chem. Soc. 2021, 143, 28, 10582–10589


M^{n+}
[M]
Lamination

Oral Presentation : **MAT.O-7**
Oral Presentation for Young Material Chemists
Room 107 THU 10:00
Chair: Jaewon Lee (Chungnam National University)

Crystal-Water-Free Potassium Vanadium Bronze ($K_{0.5}V_2O_5$) as a Cathode Material for Ca-Ion

Meladia Elok Purbarani

Energy Science and Engineering, DGIST, Indonesia

The research to discover a suitable cathode material for calcium-ion batteries (CIBs) remains challenging, despite their potential advantages of high energy density and cost-effectiveness. Herein, we report $K_{0.5}V_2O_5$ as a cathode material for CIBs. During the initial charging of the electrode, potassium ions were replaced with 0.12 Ca. The calcium-exchanged electrode exhibited a reversible discharge capacity of ~100 mAh g^{-1} at 0.1 C rate at room temperature with an average voltage ~3.0 V (vs. Ca/Ca^{2+}). The reversible capacity is higher than any reported cathode materials without crystal water, demonstrating the feasibility of further development of high-capacity crystal-water-free CIB cathode materials.

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

Oral Presentation for Young Material Chemists

Room 107 THU 10:10

Chair: Jaewon Lee (Chungnam National University)

Zeolite-templated nanoporous carbon material as iodine host for zinc-iodine battery-supercapacitor hybrid electrode

Hongjun Park, Ryong Ryoo*

Center for Nanomaterials and Chemical Reactions, Institute for Basic Science, Korea

Zinc (Zn)-based battery-supercapacitor hybrid (BSH) systems are considered a promising energy storage platform due to the low cost, safety, and high energy density compared to those of conventional lithium-based batteries. However, the development of efficient BSH electrodes is challenging due to the rise of the need for efficient supercapacitor electrodes, to solve the problem of the low power density of common batteries. Here, we report the Zn-based BSH energy storage applications using loaded iodine (I_2) species inside the pores of zeolite-templated nanoporous carbon (ZTC) for use as an electrode material. The uniform pore structure of the ZTC serves as a nanocage stabilizing I_2 to be used as a battery material, while at the same time providing a fast electron transport path through the high surface area comprised with graphene-based frameworks. By applying the prepared I_2-loaded ZTC (I_2/ZTC) electrode, it was possible to operate both Zn-based battery and BSH devices. The I_2/ZTC electrode exhibits excellent performance with ultra-high energy and power densities (111 W h kg^{-1} and 847 W kg^{-1}, respectively) along with high cyclic stability owing to the nanopores confinement effect. It is demonstrated that this combination of three-dimensionally graphene-based nanoporous material (*i.e.*, ZTC) and I_2 provides an easy way to realize economical next-generation batteries.

Oral Presentation : **MAT.O-9**
Oral Presentation for Young Material Chemists
Room 107 THU 10:20
Chair: Jaewon Lee (Chungnam National University)

An Introduction to ChemAI: Platform for Data-Driven Material Chemistry Research

Seunghun Jang*, Gyoung S. Na, Hyunju Chang

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

Machine learning (ML) has been applied to various materials research fields and achieved great results because it allows us to predict important material properties for a variety of materials rapidly. This trend has been promoted the construction of a vast material database and has influenced a positive impact on various fields of material research, such as the development of algorithms for more sophisticated predictions, optimization of experimental conditions, or material screening through it. However, these studies are mainly carried out by code-based studies of specific material-research groups. To promote material development through artificial intelligence, various material researchers should be able to create predictive models with high accuracy through simple manipulations from their own databases. ChemAI is a platform for data-driven materials research to support users to build their own predictive models with their own datasets and provides various types of toolkits implemented by advanced deep learning models.In particular, ChemAI can predict structure-based properties using material structure information such as CIF or SMILES. All ML tasks are conducted under a web-based environment, and a user interface environment has been built so that even researchers with little experience in code development can freely use them.In this presentation, I would like to introduce the main functions provided by ChemAI. We expect that ChemAI will serve as a catalyst for many researchers in the field of material chemistry to conduct advanced material research through ML.

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

Oral Presentation for Young Material Chemists

Room 107 THU 10:30

Chair: Jaewon Lee (Chungnam National University)

Size, morphology and surface charge determined biological behaviors of layered double hydroxide nanomaterials upon blood components

Tetsuo Yamaguchi, Jae-Min Oh[1,*]

Department of Energy and Materials Engineering, Dongguk university, Korea

[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Layered double hydroxides (LDHs) exist as hydrotalcite in nature and is known biocompatible nanocarrer for drugs, while the reports about the biocompatibility is limited so far. In this study, the biocompatibility of LDHs for blood components, red blood cell (RBC) and proteins, was investigated from aspects of size, morphology and surface charge of LDHs. LDHs with three sizes (lateral size: 160, 340 and 2000 nm) and three surface charges (ζ-potential: −15, 5.6 and 36 mV) were successfully synthesized, respectively. SEM revealed that a few LDH particles adsorbed on the RBCs by electrostatic interaction between the positively charged LDH and the negatively charged RBC. Hemolysis ratios by the LDHs were less than 2% which is acceptable in biomaterials, although the LDH with the lateral size of 2000 nm showed a slightly higher ratio. It was thought that the larger diameter of the LDH enabled to interact with RBC in lager contacting surface than the other LDHs.Interactions between the LDHs and blood plasma were investigated from fluorescence quenching. Blood proteins includes fluorescent amino acid, phenylalanine, tyrosine and tryptophan, where tryptophan contribute the fluorescence mainly. The fluorescence of amino acids largely depends on the molecular environment. The fluorescence quenching ratio by the LDHs with different sizes were similar (ca. 0.25), while the ratio decreased from 0.3 to 0.09 with decreasing the surface charge from positive to negative. The adsorption isotherm estimated from the quenching ratio was type III and V, investigating weak interactions of the proteins to the LDHs. The quenching behavior was explained by modified Stern-Volmer equation, suggesting that the interactions between the proteins and the LDHs included several manners.

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

Oral Presentation for Young Material Chemists

Room 107 THU 10:40

Chair: Jaewon Lee (Chungnam National University)

Understanding the Origin of the Pressure-Induced Amorphization in metal halide perovskite $CsPbI_3$

Seho Yi

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

A recent high-pressure study reported the reversible phase transition from crystal to amorphous occurs under an external pressure in metal halide perovskite, $CsPbI_3$ [1]. Here, we investigate the origin of the pressure-induced amorphization in $CsPbI_3$ using first-principle density-functional theory (DFT) calculations. According to our DFT calculations, the amorphous-like phase becomes energetically more stable than the orthorhombic crystalline phase by 12 meV over 7 GPa. Moreover, we find that the flat unstable phonon modes appear in the phonon dispersion across the Brilliouin zone at a pressure of 7 GPa. These degenerated unstable phonon modes correspond to inter and intra PbI_3 octahedral distortions. Thus, it is likely to form random-like octahedral tilting patterns under compression leading to the loss of long-range order. We believe that this is mainly responsible for the pressure-induced amorphization in $CsPbI_3$, and our findings give a deeper understanding of the underlying mechanism of the pressure-induced amorphization in halide perovskites.[1] Y. Cao, *et al.*, J. Phys. Chem. 122, 9332 (2018).

Oral Presentation : **MAT.O-12**
Oral Presentation for Young Material Chemists
Room 107 THU 10:50
Chair: Jaewon Lee (Chungnam National University)

Oxidative Coupling of Methane (OCM) using Mixed Ionic-Electronic Conducting (MIEC) Membrane

Bonjae Koo

School of Chemistry and Energy, Sungshin Women's University, Korea

The production of C2 hydrocarbons such as ethylene (C2H4) and ethane (C2H6) is important for the chemical industry. With the depletion of liquid petroleum, natural gas containing primarily methane (CH4) is expected to be one of the main resources for the C2 gas production. Oxidative coupling of methane (OCM) is an attractive route for direct conversion of methane to valuable chemicals, mainly C2 products. Nevertheless, the main barrier to commercialization of OCM is that the C2 yield is too low due to the deep oxidation of highly reactive products in operating conditions. To overcome this challenge, considerable research efforts on OCM have been devoted to the development of ion-conducting ceramic membrane. In case of OCM using the ion-conducting membrane, oxygen permeates through the ceramic membrane and reacts with the methane on the membrane surface where conversion takes place, thereby selectively avoiding partial or complete oxidation of methane.In this talk, I will present OCM for C2 hydrocarbon production using Zr-containing BaFeO3-δ membrane with lanthanum oxide (La2O3) as a catalyst in a fixed-bed configuration. BaFeO3-δ, a cobalt-free perovskite oxide, has been considered as a candidate membrane material for OCM due to its high oxygen permeability but it generally exists as a multiphase compound because of a mismatch in the ionic radius between Ba and Fe. Zr is introduced into Fe site for chemical stabilization of BaFeO3-δ in operating condition for OCM. Gas-phase analysis near the membrane is performed to suggest a global reaction mechanism for the conversion of methane to C2 products that accounts for gas-phase and surface reactions. Based on this, it is shown that OCM in a lab-scale membrane reactor is able to achieve a high yield of C2 under long-term operation without membrane degradation or catalyst deactivation.

Award Lecture in Division : **ELEC.O-5**

Oral Presentation of Young Scholars in Electrochemistry

Room 108 THU 10:30

Chair: Jinho Chang (Hanyang University)

Expanding the research area of electroanalytical chemistry: single-entity electrochemistry and polymer analysis

Byung-Kwon Kim

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Recently, single particle analysis through electrochemical collision (i.e., nano-impact electrochemistry or single-entity electrochemistry) on ultramicroelectrodes has been actively studied. This single particle collision method is a great way to analyze diffusion coefficients, single particle compositions, size distribution of particle, concentrations, and diffusion behavior of particles in solution. Our group studied soft particles such as emulsions (water/oil and oil/water), bacteria, red blood cells and platelets by electrochemical single particle collision. These studies take advantage of the increase or decrease in the current signal that occurs when a single particle collides the electrode surface. The second topic is electroanalytical chemistry for polymers. Polymers are materials closely related to our daily life, but it is difficult to analyze through electroanalytic chemistry. These are because most polymers are electrochemically inactive materials. Our research group introduces new electroanalytic techniques that analyzes the properties of these electrochemically inactive polymers by using solution viscosity and the interaction of the electrochemically active redox species.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 108 THU 09:00

Chair: Jinho Chang (Hanyang University)

Morphological effects of nanoporous Indium tin oxide electrodes towards electron transfer and its applications as bipolar electrode sensors

Minjee Seo

Department of Chemistry Education, Korea National University of Education, Korea

Fabrication of nanostructured materials in order to enhance its catalytic activity has long been indispensable in electrocatalyst development. In particular, nanoporous structured electrodes have attracted attention due to their enlarged surface-to-volume ratio, high density of surface defects and altered crystalline facets, leading to enhanced catalytic activities. In the geometrical point of view, nanocavities of nanoporous electrodes offer unique spatial environment, resulting in altered physicochemical characteristics that affect the electrocatalytic performance. For instance, it has been suggested that confinement of reactant molecules lead to enhanced interaction between the reactant molecule and the electrode, a phenomenon denoted as nanoconfinement effects. To clearly observe the nanoconfinement effects, nanoporous Indium tin oxide (ITO) electrodes were utilized to investigate the single electron transfer kinetics of Fe2+/3+. By varying the nanoporous ITO layer thickness and comparing their electrocatalytic performance, we were able to effectively exclude catalytic effects originating from the electrode surface characteristics. The catalytic effects of nanoporous ITOs were also demonstrated by its applications in bipolar based sensors.

Oral Presentation : **ELEC.O-2**
Oral Presentation of Young Scholars in Electrochemistry
Room 108 THU 09:20
Chair: Jinho Chang (Hanyang University)

Hydrogen Production on Atomically Precise Metal Nanoclusters: Effects of Foreign Metal-doping and Surface Modification

Woojun Choi

Department of Chemistry and Medical Chemistry, Yonsei University, Korea

Developing of an efficient hydrogen evolution reaction (HER) catalyst is one of the challenging field to replace the fossil fuel. Atomically precise metal nanoclusters could be promising candidates due to their distinctive electrochemical property and HER activity. They have well-defined molecular formula such as $Au_{25}(SR)_{18}$, $Au_{38}(SR)_{24}$ and $Ag_{25}(SR)_{18}$ where SR is thiolate ligand, and HER activities of nanoclusters can be considerably modified in atomic precision. In this presentation, we report promoted HER activities of Au (or Ag) nanoclusters by metal doping and surface modification. The HER features such as onset potential and turnover frequency (TOF) were demonstrated by linear sweep voltammetry and controlled potential electrolysis. Pt (or Pd) doped nanoclusters showed substantially reduced onset potential which could be understood by the electron-transfer mediator effect of doped nanoclusters exhibiting matched reduction potential with that of proton. Moreover, they exhibited enhanced current densities and TOFs of H_2 compared with the undoped nanoclusters. Density functional theory reveals that thermoneutral binding step with H^+ ($\Delta G_H = \sim 0$ eV) ensure high HER performance of doped nanoclusters. Further, the TOFs of Pt-doped nanocluster was further enhanced by surface modification via proton-relaying sulfonate ligands, leading to TOF of 100 s^{-1} at −0.6 V.

Oral Presentation : **ELEC.O-3**
Oral Presentation of Young Scholars in Electrochemistry
Room 108 THU 09:40
Chair: Jinho Chang (Hanyang University)

Interfacial Stabilization of All-Solid-State Batteries with Highly Concentrated Electrolytes

Minjeong Shin

Department of Chemistry and Energy, Sungshin Women's University, Korea

All-solid-state lithium-sulfur battery (ASSLSB) is considered a promising technology to electrify transportation due to its enhanced safety and high energy density compared to the current Li-ion battery. In addition, ASSLSB mitigates issues related to “polysulfide shuttle” present in liquid-based Li-S cells. Despite such advantages, achieving high performance ASSLSB is challenging due to poor interfacial properties at solid electrolyte/electrode interfaces. To address challenges related to poor interfacial contact, we use the strategy of modifying the interface by employing the highly concentrated solvate electrolyte as an interlayer material at the electrolyte/electrode interfaces. The incorporation of the interlayer enhances the cyclability of the solid-state Li_2S cell compared to the bare counterpart. Electrochemical impedance spectroscopy of the interlayer-modified cell shows a gradual decrease in interfacial resistance as a function of cycle number, whereas the cell impedance of the bare cell remains constant.Another way to utilize the solvate electrolyte is to premix the solvate with solid electrolyte to prepare a solvate-solid electrolyte mixture (“solvSEM”) electrolyte. The cell using solvSEM electrolyte further improves the cycling performance in terms of active material utilization, capacity retention, and active material loading. This hybrid configuration combines the benefits of solid electrolyte and solvate electrolyte in that solid electrolyte acts as a blocking layer for polysulfide dissolution and diffusion while solvate electrolyte forms the favorable ionic contact at battery interfaces.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 108 THU 10:00

Chair: Jinho Chang (Hanyang University)

Structure and properties of a superprotonic solid acid, $Cs_2(HSeO_4)(H_2PO_4)$

Ara Jo, Sossina M. Haile[1,*]

Department of Chemistry, Kangwon National University, Korea
[1]*Materials Science and Engineering, Northwestern University, United States*

We investigated a superprotonic solid acid, $Cs_2(HSeO_4)(H_2PO_4)$, which shows phase transition starting at 115 °C. The structure was studied using high temperature X-ray diffraction, which showed that the phase transition from monoclinic to cubic structure. The conductivity of $Cs_2(HSeO_4)(H_2PO_4)$ jumped with the phase transition from 1.27×10^{-4} S cm^{-1} at 115 °C to 2.81×10^{-3} S cm^{-1} at 140 °C. The dehydration which occurred at the similar temperature with the superprotonic transition with the elevated temperature was suppressed by only 0.2 atm of pH_2O and the next dehydration showed up at 260 °C, which indicated that $Cs_2(HSeO_4)(H_2PO_4)$ can be used as an electrolyte with a wide operational region of stability for solid acid electrochemical cell.

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

General Session

Room 110 THU 09:30

Chair: Wooyul Kim (Sookmyung Women's University)

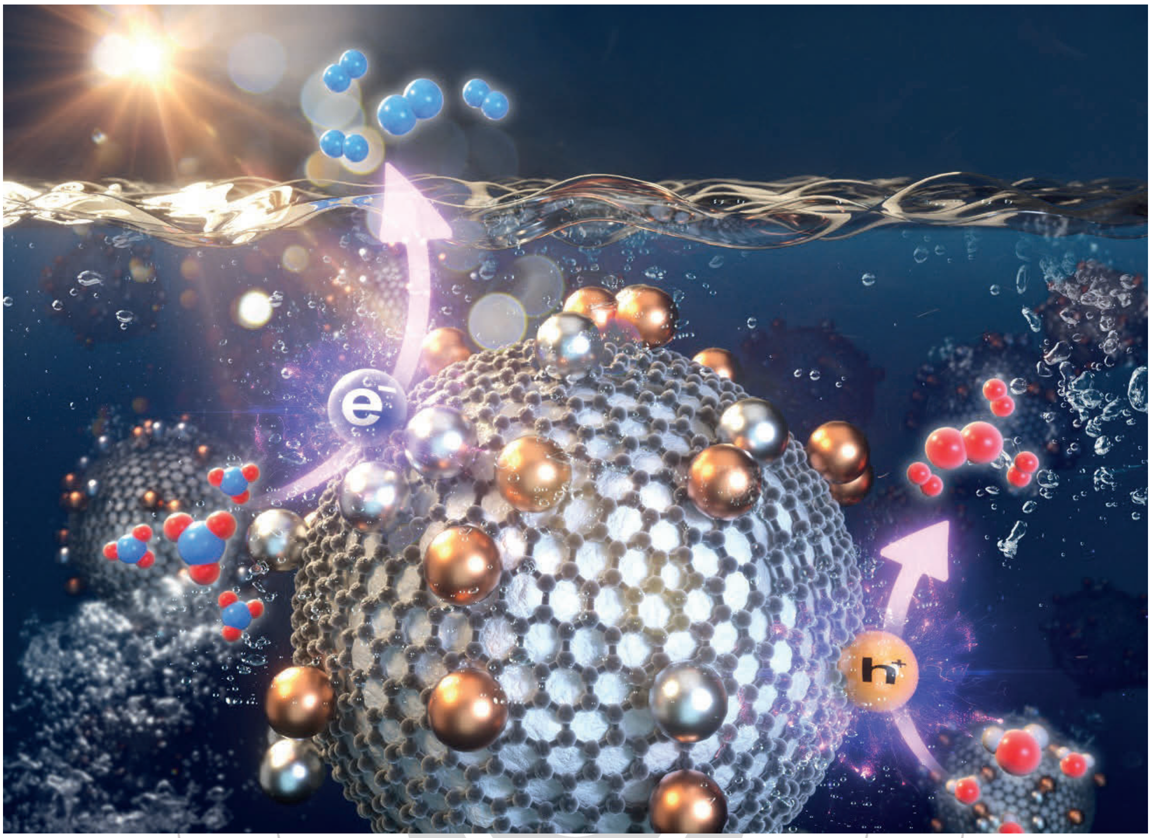
Highly selective solar denitrification by *in situ* generated H_2 on TiO_2 modified with bimetals and reduced graphene oxide

Shinbi Lee, Wonyong Choi*

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

Denitrification is an essential process that converts nitrate (NO_3^-) to harmless N_2 with returning nitrogen to the atmosphere. As a potential control method, photocatalytic denitrification has attracted interests but, achieving high conversion efficiency and selectivity to N_2 without generating harmful byproducts (*e.g.*, nitrite and ammonium) is still a challenging issue. In particular, the previous studies using co-catalysts loaded photocatalysts essentially need chemical reducing reagents such as organic compounds and H_2, which is regarded as a major bottle neck for their scalable operation. Here we propose the first example of the ‘chemical reductant-free’ solar denitrification system and develop a novel composite photocatalyst composed of TiO_2, Cu-Pd bimetals, and reduced graphene oxide (rGO) (Cu-Pd/rGO/TiO_2) to transform nitrate to N_2 with achieving near 100% conversion and selectivity to N_2 and generating little byproducts. Direct conversion of nitrate to N_2 occurs on Cu-Pd/rGO/TiO_2 by promptly consuming *in situ* generated H_2 (*via* water splitting) as a reductant while it is not possible at all with rGO/TiO_2 and Cu-Pd/TiO_2. The *in situ* water splitting on Cu-Pd/rGO/TiO_2 was confirmed by the concurrent H_2 and O_2 evolution in the absence of nitrate. The unique activity is ascribed to the synergic action of Cu as a co-catalyst for nitrate-to-nitrite conversion, Pd for nitrite-to-dinitrogen conversion, and rGO for the enhanced charge separation/transfer and H_2 production. The time-resolved photoluminescence and electrochemical characteristics of the ternary composite reveal that the co-existence of Cu-Pd and rGO significantly retards the charge recombination and facilitates the selective electron transfer to nitrate with the quantitative production of N_2. The introduction of rGO enabled the denitrification even under visible light (up to 450 nm) and apparent quantum yield (AQY) of N_2 production reached a maximum of 4.9% at 320 nm. The proposed system provides a breakthrough strategy that combines “environmental photocatalysis” with “energy photocatalysis” (H_2 production *via* water splitting) as a sustainable solution for controlling nitrogen

pollutants. **Acknowledgements** This research was financially supported by the Leading Researcher Program (NRF-2020R1A3B2079953), which was funded by the Korea government (MSIT) through the National Research Foundation of Korea (NRF).



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

General Session

Room 110 THU 09:45

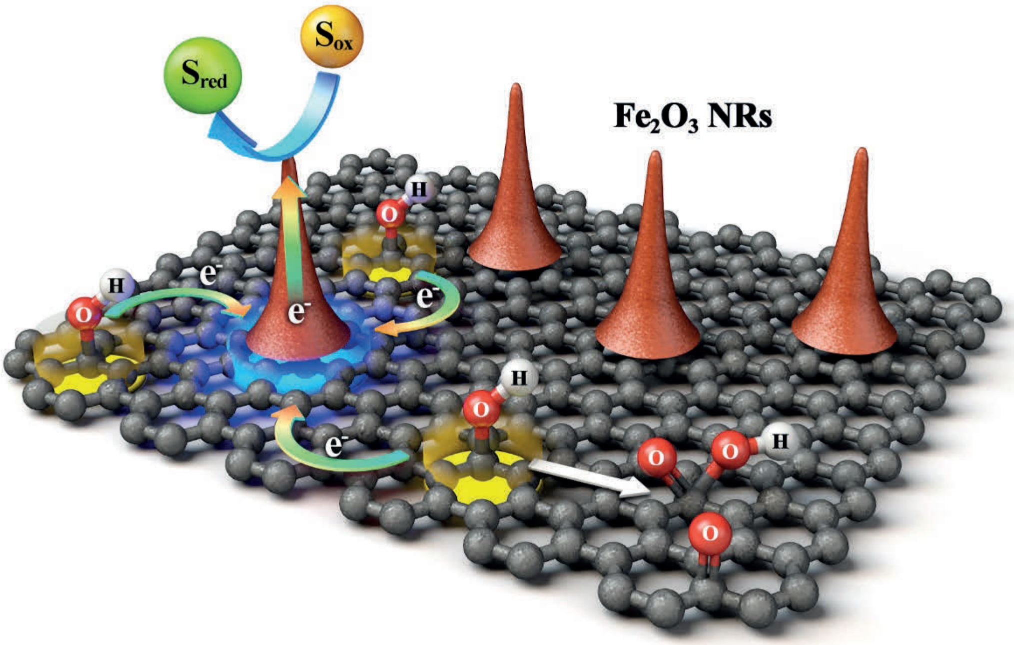
Chair: Wooyul Kim (Sookmyung Women's University)

Spontaneous reductive transformation of inorganic substances by Fe_2O_3 nanorods on carbon nanofibers under dark ambient aerated water

Chuhyung Kim, **Wonyong Choi**[1,*]

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

Fe_2O_3 nanorods loaded on carbon nanofiber sheet (Fe_2O_3/CNF) was found to be active in reductive transformation of recalcitrant inorganic substrates under dark and ambient conditions without needing any external energy or chemical oxidants. Fe_2O_3/CNF exhibited significant spontaneous reductive transformation activities for a variety of inorganic ions and transition metal ions (13 inorganic substances), whereas Fe_2O_3 or bare CNF alone exhibited negligible activity. The quantitative conversions to reduced products on Fe_2O_3/CNF were demonstrated for the cases of $Fe(CN)_6^{3-}$, IO_3^-, ClO_3^-, and BrO_3^-. The spontaneous reductive transformation was further confirmed by the cathodic current generation on Fe_2O_3/CNF electrode upon spiking target inorganic substrates. Together with several characterizations and analyses, the synergic combination of Fe_2O_3 and CNF initiated the spontaneous electron transfer from the oxygen-containing functional groups on CNF to the inorganic substrates through Fe_2O_3 nanorods. The spontaneous reductive transformation of various inorganic ions and transition metal ions on Fe_2O_3/CNF could be proposed as a novel environmental remediation technology that can reduce low-level of various pollutants.


S_{ox}
S_{red}
Fe_2O_3 NRs
e^-
e^-
e^-
e^-
e^-
O
H
O
H
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O

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

General Session

Room 110 THU 10:00

Chair: Wooyul Kim (Sookmyung Women's University)

Research on Contaminants Originated from Chemical Combustion and Metabolome in Contaminated Soil Using LC-MS based Metabolomics and 16s rRNA Genome Sequencing

Jungman Jo, Jeongae Lee[1,*], Jaeyoung Choi[2,*]

Environment, Health and Welfare Research Center, Korea Institute of Science and Technology / KOREA Univ., Korea

[1]*Molecular Recognition Research Center, Korea Institute of Science and Technology, Korea*

[2]*Environment, Health and Welfare Research Center, Korea Institute of Science and Technology, Korea*

Chemical accidents have frequently occurred due to the increasing use of chemicals in the industries. In the past, Post-Ecological Impact Assessment in soil has been performed on leakage accident rather than fire and explosion accidents since it was generally considered that most combustion gases from chemical fire and explosion disappeared into the atmosphere and did not cause soil contamination. In this study, the possibility of soil contamination by toluene fire accident was proposed. A fire simulation batch test was performed and identified the name of combustion products such as ethylbenzene, ethynylbenzene, benzaldehyde, naphthalene, 2-methylindene from toluene combustion test using GC-MS. Metabolomics based on LC–MS was also applied in this research to estimate the biological state in contaminated soil. Naphthyl-2-methyl-succinic acid, which is a metabolic intermediate of naphthalene (combustion product of toluene) was discovered including secondary metabolites such as antibiotics (streptomycin 6-phosphate), 3-nitroacrylate and oxaloacetate in soil. As a result, soil bacterial stress response in contaminated soil affected by combustion gas cloud were identified by discovering metabolites related to bacterial self-defense action such as fatty biosynthesis and activation of electron circulation. This study draws a conclusion that soil can be polluted enough to affect soil bacteria community by gas cloud and soil bacteria can encounter stress for a long term even though toluene and its combustion products had already decomposed in soil.

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

General Session

Room 110 THU 10:15

Chair: Wooyul Kim (Sookmyung Women's University)

Oxidative conversion of rhodochrosite ($MnCO_3$) to groutite (α-MnOOH) in the presence of goethite (α-FeOOH) substrate

Seonyi Namgung, Gieyeon Lee*

Department of Earth System Sciences, Yonsei University, Korea

Rhodochrosite ($MnCO_3$) is commonly found in terrestrial and marine deposits as a main sink of Mn in anoxic and suboxic environments. The oxidative conversion of rhodochrosite to Mn (oxyhydr)oxides greatly exerts control over the (bio)geochemical cycles of various substances in the environment because Mn (oxyhydr)oxides play pivotal and diverse roles as powerful oxidants and scavengers. Thereby, there have been extensive studies on the oxidation process of dissolved Mn(II) forming diverse Mn (oxyhydr)oxides. However, the oxidation of solid phase Mn(II) such as rhodochrosite has been rarely explored. This study examined the stability of rhodochrosite against oxidation by atmospheric oxygen with a special focus on the geochemical roles of goethite as a model solid substrate ubiquitous in the environment. The results showed that rhodochrosite oxidation was limited in the absence but substantially accelerated in the presence of goethite. It is noteworthy that rhodochrosite oxidation induced heteroepitaxial growth of groutite (α-MnOOH) on the goethite (α-FeOOH) tip surfaces, indicating that the goethite substrate constrained the oxidation product. This process catalyzed rhodochrosite dissolution by generating protons in the vicinity of rhodochrosite particles. These results shed light on the critical role of foreign solid substrates on the geochemical stability of redox-sensitive solid phases in the environments.

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

General Session

Room 110 THU 10:30

Chair: Wooyul Kim (Sookmyung Women's University)

Single-atom Sn-Cu/C_3N_4 catalyst for selective solar synthesis of HCHO from CO_2

Bupmo Kim, **Wooyul Kim[1,*]**, **Wonyong Choi[2,*]**

Department of Chemical Engineering, Pohang University of Science and Technology, Korea
[1]*Department of Chemical and Biological Engineering, Sookmyung Women's University, Korea*
[2]*Division of Environmental Science and Engineering, Pohang University of Science and Technology, Korea*

Single-atom catalysts have been used in various catalysis research. Due to their high selectivity and activity, single-atom catalysts are one of the promising candidates to produce the value-added chemicals from CO_2 gas. However, it is still challenging to produce formaldehyde due to its instability. Here we synthesis formaldehyde from CO_2 reduction reaction using single-atom Sn-Cu/C_3N_4 photocatalyst. Sn(II) and Cu(I) coordination with nitrogen of C_3N_4 occurred through the one-pot annealing process. Sn(II) and Cu(I) single-atom enable to stabilization of formaldehyde intermediates. In addition, in-situ liquid transmission infrared absorption spectroscopy measurements were carried out to trace C=O and C-H bonds of formaldehyde. Furthermore, $^{13}CO_2$ isotope labeling experiments are also conducted to confirm the carbon source. Our investigation will provide a platform for understanding of single-atom photocatalyst and formaldehyde production.

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

General Session

Room 110 THU 10:45

Chair: Wooyul Kim (Sookmyung Women's University)

Water-compatible conjugated polymer photocatalysts by side-chain engineering

Jeehye Byun

Water Cycle Research Center, Korea Institute of Science and Technology, Korea

Conjugated polymers have emerged as a new class of heterogeneous photocatalysts for utilizing visible light as an environmentally friendly energy source. By virtue of structural designability, the conjugated polymers can be tuned to show better hydrophilicity by side-chain engineering particularly for targeting the photocatalytic reactions in an aqueous medium, e.g. photocatalytic degradation of contaminants, water splitting, and photoredox reactions in water. We have designed a linear chain conjugated polymer to have different terminal functionalities such as diethylamine (DEA) and vinylimidazole (Vim) for initiating a reversible wettability change. The DEA-based conjugated polymer exhibited reversible hydrophilicity in the presence of CO_2 gas as the tertiary amine captured CO_2 molecules with water to form ammonium-bicarbonate salt, making the whole polymers hydrophilic for improving photocatalytic activity in water. Once the CO_2 was detached, the polymer could be easily separated from water for recycling. In the case of Vim-terminated conjugated polymer, the polymer chain could be transformed into nanoparticles or incorporated into membranes and hydrogels through free-radical polymerization of the vinyl group, leading to generate a series of hydrophilic photocatalytic platforms. The reversible wettability control of the Vim-based structures was achieved by a simple ionic exchange protocol. The utility of the photocatalytic platforms was demonstrated in the environmental applications under visible light illumination, such as water treatment, bacterial disinfection, and oxidation of NADH enzyme cofactor.

Poster Presentation : **POLY.P-1**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Metal-Mediated Approach to Grafting Zwitterionic Polymers onto Solid Surfaces for Non-Biofouling Applications

Yohan Kim, Yejin Kim[1], Woo Kyung Cho[2], Joon Sig Choi[3], Sung Min Kang[4,*], Minjin Seong[2]

chemistry, Chungbuk National University, Korea
[1]*Chungbuk National University, Korea*
[2]*Department of Chemistry, Chungnam National University, Korea*
[3]*Department of Biochemistry, Chungnam National University, Korea*
[4]*Department of Chemistry, Chungbuk National University, Korea*

Hydrophilic polymer coating on solid surfaces has been of interest because it prevents nonspecific adsorption of biomolecules onto solid surfaces. Among the various hydrophilic polymer coatings, zwitterionic polymer coating has gained a great deal of attention, due to the exceptional hydration capability through ion-dipole interactions. Much effort has been made to develop an efficient method for grafting zwitterionic polymers onto solid surfaces. However, previous methods showed limitations that a large amount of reagents or a time-consuming process is required for grafting zwitterionic polymers. Herein, we propose a facile strategy for zwitterionic polymer coatings, namely, coordination-driven zwitteration. Mussel-inspired polydopamine is used as an intermediate layer and the zwitterionic polymers are then grafted on the polydopamine-coated surface via coordinate bond formations. Zwitterionic polymer-grafted surfaces are very hydrophilic and highly resistant to protein adsorption and bacterial adhesion.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Development and evaluate of genistein encapsulated polymeric micelle using biocompatibility polymer

나래(Narae) 박(Park)

New Drug Discovery and Development, Chungnam National University Graduate School of New Drug Discovery and Development, Korea

Used in this study, the genistein is a phytoestrogen and has antioxidant and wrinkle improvement efficacy. However, the material is having difficulty developing materials due to low solubility. The purpose is to develop polymeric micelle using biocompatibility polymers for encapsulation and to evaluate stability, particle size, skin permeability, and efficacy.Long-term stability test was performed by HPLC, particle size was analyzed by ELS-Z, and skin permeability was performed by Franz diffusion cell for 24 hours. Also, an in vitro test was proceeded.As a result, developed polymeric micelle were stable for six months, and the particle size was 20 to 80 nm, and the skin permeability was about 8 %. The efficacy of nanoparticles for antioxidants and wrinkle improvement were confirmed by in vitro test results.Therefore, it is expected that developed polymeric micelle can be applied to various formulations.This study was carried out with the support of the Ministry of SMEs and Strartups(Project No:S2917267).

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Preparation of Organic-Inorganic Hybrid Biodegradable Polyesters Containing Fertilizer Ingredients

Hyun Ju Lee, **Bun Yeoul Lee**[1,*]

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

Polyesters produced through the condensation reaction of a diol (eg, 1,4-butanediol) and a dicarboxylic acid (eg, succinic acid, adipic acid, and terephthalic acid) are biodegradable polymers. Because of the persistent environmental problems of plastics, the current public and industrial interest in such biodegradable polymers is considerable. Typically, a condensation reaction is performed using titanium alkoxide as a catalyst, but there is a limit to increasing the molecular weight. Therefore, after the condensation reaction, a chain linker such as diisocyanate is additionally added to increase the molecular weight of the resulting condensate. A method for preparing a biodegradable polyester having high viscosity and mechanical strength without using a titanium alkoxide catalyst, instead of using a phosphoric acid as a catalyst, without adding a chain linker will be disclosed. And a method for producing a biodegradable polyester having a new structure and composition is disclosed.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Polymer-Metal-Composite-Type Electrodes for Flexible Solar Cell Applications

Jong Jin Park, Jong Hyun Kim*

Department of Molecular Science and Technology, Ajou University, Korea

- Withdrawal -

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Aluminium sensitive Rhodamine-bearing poly(2-isopropyl-2-oxazoline).

Chanho Shin, Woo-Dong Jang[*]

Department of Chemistry, Yonsei University, Korea

Rhodamine 6G-bearing telechelic poly(2-isopropyl-2-oxazoline) (R6G-PiPrOx-R6G) was designed and synthesized for selective recognition of Al^{3+}. The fluorescence of R6G-PiPrOx-R6G in aqueous solution turned on in respond to Al^{3+}. The color of solution was changed to pink upon addition of Al^{3+}. The cloud point of temperature was also changed by Al^{3+} binding into the polymer. Furthermore, R6G-PiPrOx-R6G formed polymeric micelles in aqueous solution with a critical micelle concentration of 0.042 g/L and the micelles were disassembled by Al^{3+} due to the increasing hydrophilicity. The R6G-PiPrOx-R6G has a potential for drug delivery system using Al^{3+}-sensitive properties.

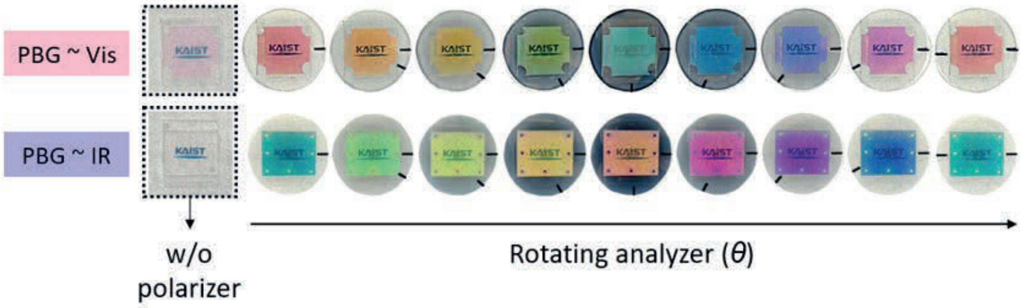
Poster Presentation : **POLY.P-6**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Structural Color Changes by Engineering Optical Rotation of Chiral Photonic Crystal

Wongi Park, Hyewon Park[1], Dong Ki Yoon[1,*]

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

Photonic crystals (PC) are periodic dielectric structures, and they have structural colors by reflecting a specific wavelength of light, also known as photonic bandgap (PBG). In chiral PC, there is optical rotation (β), in which the polarization axis of linearly polarized light rotates when it enters the chiral medium. The optical rotation diverges at PBG wavelength due to the photonic resonance effect and decreases in proportion to the square of the inverse of the wavelength at wavelengths much shorter than the PBG region. Also, there is optical rotatory dispersion in which optical rotation dramatically varies with the wavelength, which becomes a driving force for color changes. The optical rotation-based structural color changes can be achieved by positioning the chiral PC film between polarizer and analyzer and rotating an analyzer. Herein, we show a structural color tuning method that depends on the optical rotation and PBG wavelength using cholesteric liquid crystals. The concentration of chiral dopant can easily control the PBG wavelength. As a result, we can precisely engineer PBG wavelength and optical rotation, enabling the optical rotation-based structural color changes. The various colors can be expressed within one PC film by simply rotating the analyzer, and the color gamut is different depending on the position of the PBG wavelength. Moreover, when the PBG wavelength is located in IR range, this PC film can control the transmission of a specific wavelength to 0% while remaining transparent. We developed an active type protective goggle using this characteristic, and various wavelengths are blocked according to the rotation angle. We expect these optical rotation-based structural color changes can be applied in the more advanced optical technology.


PBG ~ Vis
PBG ~ IR
KAIST
w/o polarizer
Rotating analyzer (θ)

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Supramolecular chemistry based porphyrin catalysts

Yeongchan Seo, Kyeong-Im Hong, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Poly(3-hydroxybutyrate) (P3HB) produced by bacteria is biodegradable and eco-friendly polymer. Its properties show the potential to replace petroleum plastics. Currently, chemical synthesis of P3HB is being conducted in solution polymerization, but from the stand of industrial application, bulk polymerization has several advantages such as low cost, eco-friendly and advantages of management and technical production. In the previous work, ring opening polymerization (ROP) of racemic β-butyrolactone (*rac*-BBL) was successfully conducted in the presence of porphyrin and proton sponge. Based on this result, we suggested various Zn porphyrins for homogeneous and heterogeneous catalysts in bulk polymerization. By changing the aldehyde of porphyrin precursor, we prepared catalyst that highly soluble in monomer as well as heterogeneous catalyst. Using heterogeneous catalyst, P3HBs were formed with M_n up to 18000 g·mol^{-1}. On the other hand, using homogeneous catalyst, P3HBs were formed with M_n up to 36800 g·mol^{-1}.

Poster Presentation : **POLY.P-8**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis of Monodisperse Brush Polymer

Hyunji Ma, Kyoung Taek Kim[*]

Division of Chemistry, Seoul National University, Korea

Bottlebrush polymers possess densely grafted side chains on a long linear backbone. Owing to the distinct structure of these bottlebrush polymers, the properties and behavior of polymers tend to differ from common linear polymers. Thus, bottlebrush polymers have become a significant focus of polymer research. However, the absolute characterization of structural parameters, composition, and purity for bottlebrush polymers has been limited due to their chemical complexity. The synthesis of monodisperse oligomers or linear polymers with defined sequences has been actively developed via the iterative exponential method. However, the synthesis of polymers with high molecular weight has not been achieved. Here, we synthesized the absolutely defined monodisperse brush polymers with monodisperse linear polymer as pendants attached to a monodisperse poly(hydroxy acid) backbone. Owing to the monodisperse backbone chains containing functional groups, the functionalization of the backbone chains with various linear side chains could be achieved via thiol–ene “click” chemistry.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Self-assembly of Oppositely Charged Ionic Block Copolymer Complex with Discrete Molecular Weight

Junyoung Kim, Mo Beom Koo, Kyoung Taek Kim[1,*]

chemistry, Seoul National University, Korea

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

When the oppositely charged amphiphilic molecules are mixed, they self-assemble to unusual structures via self-organization due to the electrostatic interactions. Oppositely charged block copolymers have seldom been used to mimic such behavior due to the synthetic difficulty and ill-defined chemical structures. Here we report the self-assembly of oppositely charged ionic block copolymer complex to highly ordered structures. We used the convergent method to synthesize monodisperse and precisely defined block co-oligomers (BCOs) having the tetramers of L-malic acid or (s)-4-amino-2-hydroxybutyric acid as a hydrophilic block and oligo(lactic acid) as a hydrophobic block. These oppositely charged BCOs, with an absolutely defined number of cations or anions were mixed in varying ratios for the co-assembly in water. The resulting self-assembled structures were characterized by electron microscopy.

Poster Presentation : **POLY.P-10**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Semi-automated synthesis of sequence-defined polymers for information storage and macromolecular engineering

Jeong Min Lee, SooJeong Lee[1], Kyoung Taek Kim[2,*]

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

Accelerated and parallel synthesis of sequence-defined polymers is an utmost challenge for realizing ultra-high-density storage of digital information in molecular media. Here we report step-economical synthesis of sequence-defined poly(L-lactic-co-glycolic acid)s (PLGAs) using continuous flow chemistry. A reactor performed the programmed coupling of the two-bit storing building blocks to generate a library of their permutations in a single continuous flow, followed by their sequential convergences to a sequence-defined PLGA storing 64 bits in four successive flows. We demonstrate that a bitmap image (896 bits) can be encoded and decoded in 14 PLGAs using only a fraction of the time required for an equivalent synthesis by conventional batch processes. Accelerated synthesis of sequence-defined polymers could also contribute to macromolecular engineering with precision comparable to natural precedents.

Poster Presentation : **POLY.P-11**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

On-demand shape transformation of polymer vesicles via site-specific isomerization of hydrazone photoswitches in monodisperse hydrophobic oligomers

Valene Wang, Kyoung Taek Kim[1,*]

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

The shape control of nanostructures formed by the solution self-assembly of block copolymers is of significance for drug delivery. In particular, site-specific perturbation resulting in the conformational change of the hydrophobic block has attracted considerable attention because of the possibility of creating polymer vesicles capable of releasing cargo molecules on demand by responding to specific stimuli. Herein, we report the synthesis of amphiphilic block copolymers based on the monodisperse molecular-weight oligo(phenyllactic acid) (OPLA) having hydrazone photoswitches at specific locations. Upon light irradiation, the photoswitch undergoes E-Z isomerization, resulting in the conformational change of the OPLA block. Polymer vesicles composed of these block copolymers exhibited reversible shape transformation upon irradiation with UV or visible light due to the E-Z isomerization of the photoswitch. Furthermore, the location and the number of hydrazone photoswitches in the monodisperse OPLA block are the decisive factors for the reversible shape transformation of the polymer vesicles from an isotropic to an anisotropic morphology.

Poster Presentation : **POLY.P-12**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Surface-initiated RAFT terpolymerization under ambient conditions

Ji Hoon Lee, Hyun Ji Seo, Seung Yeon Lee[1], Woo Kyung Cho, Kyung-sun Son[*]

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

Alkylborane compounds enable the various type of monomers can be polymerized via free radical polymerization. We investigated this organoborane-mediated polymerization method to be performed under ambient and oxygen tolerant conditions using surface-initiated reversible addition-fragmentation chain transfer (SI-RAFT) polymerization; this polymerization method is called O_2-SI-RAFT polymerization. In order to confirm the chain extension ability of RAFT polymerization, a triblock terpolymer brushes were grown on a silicon substrate via O_2-SI-RAFT polymerization. Various terpolymers on surface was analyzed by ellipsometry analysis, water contact angle analysis, X-ray photoelectron spectroscopy, and atomic force microscopy.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **POLY.P-13**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Sustained release of donepezil-loaded PLA microspheres containing latic acid.

Jihyang Lim

Department of Applied Pharmacy, Chungbuk Natioanl University, Korea

Donepezil, a choilinestserase inhibitor is one of the most widely used drugs for the treatment of Alzheimer’s disease. Donepezil-loaded PLA microspheres have a problem called ‘Initial burst release’ in which the drug is rapidlly released for 5-7 days. The purpose of this study is to optimize the sustained release of donepezil from PLA microspheres by adding latic aicd as a release retardant. PLA microspheres were prepared by O/W emulsion solvent evaporation method. The microspheres were prepared with various parameters such as drug contents and the ratio of lactic acid. Quantitative analysis was performed using HPLC. Morphological properties were analyzed by optical microscope and scanning electron microscopy. Release behavior was performed by in vitro test. As a result, the initial release inhibition is improved as the higher ratio of lactic acid and the lower initial drug content. Therefore, PLA microspheres loaded with donepezil containing latic acid have potential for long-term therapeutic effect in the treatment of Alzheimer’s disease.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Study on Synthesis and Properties of Conjugated Copolymers Containing Aromatic Heterocyclic Compound with Trifluorocarbon and Chalcogens

Nam wook Kim, Intae Kim[1,*]

Department of Chemistry, KWANG WOON university, Korea
[1]*Department of Chemistry, Kwangwoon University, Korea*

Conductive polymers are one of the research fields that are receiving a lot of attention because their applications such as solar cells, LEDs, semiconductors, and OFETs are very wide. In particular, a conductive polymer having a low band gap has properties that can be applied to an organic solar cell, so research is being actively conducted in the relevant application field. On the other hand, conductive polymers including group 16 elements, chalcogen elements (oxygen, sulfur, selenium, tellurium), have been studied in various fields. When looking at the spectroscopic and electrochemical properties of each polymer copolymerized by designing chalcogenophene (furan, thiophene, selenophene, tellurophene) in the monomer, as the size of the chalcogen group atoms increased ($O < S < Se < Te$), It has been reported that the band gap of polymers is narrowed. In this study, monomers containing thiazole and selenazole with trifluorocarbon were synthesized using various organic synthesis reactions, and electron-receiving monomers and electron-donating monomers were used for the Stille cross-coupling reaction. Conductive polymers were synthesized and their properties were compared. For each compound, structures and functional groups were analyzed using 1H NMR, 13C NMR and FT-IR. UV-vis spectrometer, Cyclic Voltammetry, Gel Permeation Chromatography, and Thermogravimetric Analysis methods were used to measure the physical properties of the polymerized polymer.Keywords : conducting polymer, solar cell, low band gap, chalcogen

Poster Presentation : **POLY.P-15**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis of cyclic diblock copolymers with discrete molecular weights

Seul Woo Lee, 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. Recently, we reported iterative convergent synthesis of large cyclic polymers with discrete molecular weights. Here, we report the synthesis of discrete linear and cyclic block copolymers. Lactic acid and chlorolactic acid were used to synthesize discrete homopolymers and alternating copolymers. The resulting discrete polymers were linked to form diblock copolymers, followed by functionalization of chain ends for the copper-catalyzed azide-alkyne cycloaddition. The resulting linear and cyclic block copolymers were purified by using preparative size-exclusion chromatography and analyzed by NMR, DSC, MALDI-TOF. We describe the effect of molecular weight fractions, molar ratio and topology of the polymer chains on the morphology of the self-assembled structures of these monodisperse block copolymers.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Polymer brush growth on various substrates using open-to-air RAFT polymerization

Minki Cho, Hyun Ji Seo, Ji Hoon Lee, Woo Kyung Cho*, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

We synthesized polymer brushes with O_2-mediated surface-initiated reversible addition–fragmentation chain transfer on various substrates using mussel-inspired surface chemistry under ambient conditions. This method allowed successful polymerization of a variety of monomers including acrylamide, methacrylate, and methacrylic acid. Characterization of polymer brushes, block copolymerization, and its application to large surfaces will be discussed in this presentation.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Effect of functional groups at hydrophilic block ends on the block copolymer self-assembly

Sungmin Ha, Kyoung Taek Kim[1,*]

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

Herein, we investigated the self-assembly behaviors of poly(ethylene glycol)-*b*-polystyrene (PEG-*b*-PS) having different functional groups at the PEG chain ends. Hydrophilic PEG blocks with methoxy, hydroxyl, and azide groups at the PEG chain ends were coupled with polystyrenes via copper-catalyzed azide–alkyne cycloadditions (CuAAC) or amidation to form block copolymers (PEG-*b*-PS). Also, PEG-*b*-PS with amine groups at the PEG chain ends was obtained via reduction of PEG-*b*-PS with azide groups. Thus produced block copolymers with a similar block ratio were self-assembled in solution to demonstrate the effect of the functional groups on the self-assembled morphologies.

Poster Presentation : **POLY.P-18**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Preparation of monodisperse Eu-Labelled Polystyrene Particles by Nanoprecipitation Method

Yoolee Lee, Daewon Sohn*

Department of Chemistry, Hanyang University, Korea

A technique called mass cytometry allows 40 cells to be separated simultaneously at a time, which requires each cell to have a lanthanide marker. Since labelled cells are nebulized and flow to argon plasma, which ionizes the metal-labelled antibodies. Then the metal signals are analyzed by a TOF (time-of-flight) mass spectrometer. For cell counting, internal standards are necessary. The particles should be suitable for mass cytometry calibration as internal standards. To perform these roles, metal-labelled microspheres were required to have monodispersity, functionality and metal content criteria. The material of the bead particle is selected as polystyrene, which can be applied in many ways, and is easily synthesized, stable, and can be made into various forms as well as applying various functional group to the surface, making it suitable for cytometry's standardization bead. In this study, polystyrene based smaller particles with quantified concentration has been studied for further application in bioanalysis. Polystyrene particle containing lanthanide metal such as Eu is fabricated by nanoprecipitation polymerization for making more monodisperse particles. The size and the morphology of the synthesized beads have been characterized by dynamic light scattering (DLS) and scanning electron microscope (SEM).

Poster Presentation : **POLY.P-19**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Preparation and Characterization of a Solution-based TiO_2-Polyimide Composite for High-k Dielectric

Jae Kyung Lee, Taek Ahn*

Department of Chemistry, Kyungsung University, Korea

The development of high performance flexible electronics requires dielectrics possessing a high dielectric constant and enhanced mechanical stability. In this study, we have developed novel solution-based TiO_2-polyimide composite dielectric based on TiO_2 precursor as a dopant in cross-linkable polyimide (PI). Polyimide (DOCDA-6FHAB) was synthesized using the monomers, 5-(2,5-dioxytetrahydrofuryl)-3-methly-3-cylohexene-1,2-dicarboxylic anhydride (DOCDA) and 5,5'-(perfluoro propane-2,2-diyl)bis(2-aminophenol) (6FHAB). And then, we introduced TiO_2 precursor to make a high dielectric constant polyimide nanocomposite layer. Polyimide nanocomposite bilayer film showed high dielectric constant (>6) and low leakage current density (1.05×10^{-5} A/cm^2 at 1 MV/cm) in metal-insulator-metal (MIM) devices. Detailed synthetic routes of polyimide and nanocomposite film fabrication condition will be presented.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Triazole Based Cross-linked Polyimide as Gate Dielectric for Low Temperature Processable Organic Thin Film Transistor

Jae Kyung Lee, Taek Ahn*

Department of Chemistry, Kyungsung University, Korea

Organic thin film transistors (OTFTs) for flexible devices require low temperature processing. We report a new cross-linker, 1,3,5-tris(2-propynyloxy)benzene (TYB), which can be cross-linkable at very low temperature 100 ^{o}C. Firstly, azide functionalized soluble polyimide is synthesized, and then cross-linking occurs through azide-alkyne cycloaddition reaction with a 1,3,5-tris(2-propynyloxy)benzene (TYB) cross-linker. The metal-insulator-metal (MIM) devices show that they show very low leakage current density (3.09×10^{-8} A/cm^2 at 1 MV/cm) and dielectric constant (3.42) even when cross-linked at very low temperature. Also, it shows good mobility (0.404 cm^2/Vs) and high on/off current ratio (1.25×10^5) through the pentacene TFT. Detailed polyimide synthesis method and film fabrication condition will be presented.

Poster Presentation : **POLY.P-21**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Applications and electropolymerization of a new thiazole derivative bearing thiophene

Joon Ho Yoon, Seunghyun Jeong, Intae Kim*

Department of Chemistry, Kwangwoon University, Korea

Conducting polymers have used as wide applications such as solar cell, battery cell, transistor, and organic light-emitting diodes. Each of the applications depend on their processing characteristics: charge transport, redox properties, and the doping level. Electropolymerization is one of the methods that used for preparing conducting polymer because of simplicity, rapidity, and reproducibility. Polymers based on thiophene is a unique aromatic heterocycle, which is electron rich. Thiophene-based conducting polymers often showed high temperature stability, potentially very high electrical conductivity and low bandgap. These characteristics make it suitable for solar cells. Research is studying on improved capacitance to make better solar cell. The larger the area, the better capacitance we get. In this study, a new monomer thiazole derivative bearing thiophene was synthesized and electropolymerized at glassy carbon and gold electrodes. The deposited polymer layers were made up by cyclic voltammetry at several scan rates, which showed superior specific capacitance and electrochemical stability. The specific capacitance and electrochemical stability can be seen by current density and galvanostatic charging-discharging curve.

Poster Presentation : **POLY.P-22**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

M^{+3}-Urushiol Combination properties study

Jun Tae Kim, Jongok Won[*]

Department of Chemistry, Sejong University, Korea

Lacquer obtained from natural lacquer trees is a natural material that can be used in various fields such as paints and adhesives for lacquerware and furniture. The main component of this lacquer is catechol derivatives substituted with various alkyl groups including double bonds. Molecules with catechol groups have the property of forming coordination bonds with metal ions. Experiments were conducted to form coordination bonds with +3-valent metal ions(M^{+3}) and urushiol, such as Fe^{+3} and V^{+3} . Using urushiol extracted from natural lacquer and, $FeCl_3$, vanadium(III) acetylacetonate ($V(Acac)_3$), the solvent used N-Methyl pyrrolidone. The presence or absence of bond formation between Urushiol and +3-valent metal ions, the combination according to the ratio was confirmed by UV-Visible Spectroscopy. M^{+3} /urushi organic gel was synthesized, the properties of the organic gel according to the concentration and ratio were confirmed, and the correlation was studied.This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No. 2020R1A2C1003562).

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Study on Synthesis and Properties of New Conjugated Chalcogenophene Monomer and Polymers Containing Fluorine

Soyeon Kim, Intae Kim*

Department of Chemistry, Kwangwoon University, Korea

Polymers containing Carbon-Fluorine bond have high thermal stability, chemical inertness to acids and bases and excellent oxidation stability. These polymers are used in various fields such as cosmetics, solar cells, biosensors and Storage cells. Heterocyclic compounds with chalcogenophene unit including group 16 elements showed various properties by thermal and optical stimulation. In particular, conducting polymers including chalcogenophene are used for optical and electrical devices due to its excellent photoelectric conversion properties. In this study, new monomers containing chalcogenophene (thiazole, selenazole) and fluorine were synthesized using various organic synthesis reactions. New conducting polymers were made by Stille cross-coupling reaction with electron-donating monomer and these new monomers. The new polymers were characterized by 1H NMR, 13C NMR, UV-vis spectrometer, Cyclic Voltammetry, and Gel Permeation Chromatography.Keywords : conducting polymer, chalcogenophene, fluorine

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

A Study on the Adhesion Properties of Fe^{3+}/Urushi/γ- Butyrolactone Organic Gel

Minseok Kim, Jongok Won[1,*]

Chemistry, Sejong University, Korea

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

The catechol derivative, natural material, urushiol, forms a multi-network through chemical bonding and additional coordination by Fe^{3+} ions. In this study, the reversibility properties of Fe^{3+}/urushi organic gels in which networks were formed in γ-Butyrolactone(GBL) solvents were identified and the adhesive properties were observed using them. Organic gels of various urushiol:Fe^{3+} molar ratios were synthesized and reversibility was measured with a rheometer. As the gelation reaction time increased, the shear modulus increased. The Fe^{3+}/urushi/GBL organogel with 70 wt% urushiol:Fe^{3+} mol ratio of 3 showed reversibility even after 3 days after the gel was formed. In addition, the 50wt% organic gel of the same mol ratio showed reversibility even after 18 days. It was confirmed that the reversibility of Fe^{3+}/urushi/GBL organic gel can be applied by measuring the tensile strength of the re-adhesive gel.This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (No. 2020R1A2C1003562).

Poster Presentation : **POLY.P-25**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Electro-Mechano-Chemically Responsive Supramolecular Switches on Mesoporous Silica Nanoparticles and their Application for Controlled Cargo Release

Gyeonghyeon Choi, Chiyoung Park*

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

Multi-responsive nanovehicle for controlled drug release have been intensively studied in biomedical application because of therapeutic efficiency. Multifunctional gate keepers on mesoporous silica nanoparticles (MSNs) have attracted substantial attention in the area of drug delivery due to high surface area, large pore volume, and good biocompatibility. However, these MSNs require complicated synthesis process in response to external physical or chemical stimuli. Here, we report facile method for synthesizing multi-responsive gatekeepers and gel composites through metal-phenolic network. Robust metal-phenolic complex showed efficient capping property without sustained release and pulsatile release of guest molecules in response to ultrasound and electrical input. This study can be realized as a promising and flexible platform for active-type drug-delivery applications such as transdermal patches and implantable gels.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Study on porous materials using chitosan with functional group of urushiol

Hyeongsu Kim, Jongok Won[1,*]

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

Modified chitosan (MC) with catechol groups which is the main component of the natural urushiol, was synthesized and used for the template for the porous materials. MC/chitosan mixed solution with different concentration was immersed in the presence of Fe^{3+} aqueous solution. Crosslinked MC/chitosan composite was prepared by the chemical and coordination bond due to the presence of Fe^{3+} ions. Porous MC/chitosan was fabricated by the freeze-drying process. The morphology and porosity were observed, and the relationship between the concentration and the porosity of the MC/chitosan was studied.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Enhancement of Mechanical Strength and Osteoconductivity of Acrylic Bone Cement by Incorporation of Hypo-crystalline PMMA Powder and Bioactive Glass 45S5

Myung Soon Hwang, Youngjong Kang[*]

Department of Chemistry, Hanyang University, Korea

The poly(methyl methacrylate) (PMMA), mainstream substance used for commercial acrylic bone cement (ABC), have intrinsic characteristics such as biocompatibility, easy processability, and high mechanical strength. In this study, we substituted pristine PMMA powder with hypo-crystallized-PMMA(hc-PMMA) powder and bioactive glass 45S5. The unique nanostructure and high modulus of the hc-PMMA itself have enhanced the compressional strength of resulting bone cement. Due to the high surface area and internal strain formed by the crystallization process, the addition of hc-PMMA dramatically decreased the polymerization time without any additional catalyst. Finally, the resulting bone cement showed high osteoconductivity than the pristine ABC composite, confirmed by the simulated body fluid (SBF) test. Based on the results, hc-PMMA and bioactive glass 45S5 incorporated bone cement can be an optimal candidate for the long-term fixation of the load-bearing implants.

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

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Ice recrystallization inhibition activity of Poly(L-Ala-co-L-Lys) (PAK)

Soyeon Park

Zhengyu Piao, Soyeon Kim, Seyeon Kim and Byeongmoon Jeong, Ewha Womans University, Korea*

Antifreeze (glycol) proteins (AF(G)P) exist in organisms that polar or subpolar areas of the ocean, and these trace amounts of antifreeze proteins cause the organism survive in lowtemperature environments. This protein binds to the ice surface to prevent ice recrystallization inhibition (IRI). In this study, PAK was synthesized by ring opening polymerization of the ε-carboxybenzyloxy-l-lysine-N-carboxy anhydrides (NCA-Kz) and l-alanine-N-carboxy anhydrides (NCA-A) in the presence of 2-amino enthanol. ε-Carboxybenzyloxy-l-lysine groups of the polymer were deprotected in trifluoro acetic acid/bromic acid in acetic acid. Analytical methods of Nuclear Magnetic Resonance Spectroscopy (NMR), Gel Permeation Chromatography (GPC), Circular Dichroism (CD) were used to identify characteristics such as chemical composition, proportion of residual monomers, molecular weight, polydispersity and ellipticity of the PAK. In particular, a significant differences in the IRI activity of poly(L-Ala-co-L-Lys) (PAK) were observed based on the ratio of Ala/ Lys and the molecular weight of PAK.

Poster Presentation : **POLY.P-29**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication of Fe(III)-Dextran Layer for Enhanced Deposition of Fe(III)-Tannic Acid Nanofilm

Hyunjung Lee, Yehee Han, Ji Hun Park[*]

Department of Science Education, Ewha Womans University, Korea

Surface modification of Fe(III)-tannic acid (TA) nanofilm incorporating various materials such as polydopamine, silica ($\mathrm{SiO2}$), and eggshell membrane hydrolysate (ESMH) has been studied. However, little attempts were made to tune fundamental Fe(III)-TA nanofilm properties. We demonstrate a Fe(III)-dextran nanocoating method that serves as a boosting layer for enhanced deposition of Fe(III)-TA complex nanofilm. The fabricated nanofilms were characterized by spectroscopic ellipsometery for thickness measurement, X-ray photoelectron spectroscopy (XPS) for atomic composition analysis, atomic force microscopy (AFM) for topography analysis, and UV-vis spectroscopy for nanofilm deposition monitoring. Compared with the conventional Fe(III)-TA nanofilm deposition, Fe(III)-TA layer deposited on Fe(III)-Dextran layer showed maximum three times enhanced deposition and rougher surface. The enhancement effect disappeared at a certain concentration point of Fe(III) ($\mathrm{FeCl3 \cdot 6H2O}$) due to its acidic environment, implying that the concentration of Fe(III) in the Fe(III)-dextran coating solution is closely related with deposition thickness of Fe(III)-TA nanofilm. The experimental findings not only provide deeper understanding of metal-polyphenol complex nanofilm deposition, but also contribute to organic nanocoating field employing polysaccharides and polyphenol combinations.

Poster Presentation : **POLY.P-30**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Resveratrol-β-Lactoglobulin Complexes Nanocoating with Fe(III)-Tannic acid for Enhanced Chemostability

Yeon Seo Cho, Ji Hun Park[1,*]

Department of Pharmaceutical Engineering, Dankook University, Korea

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

Resveratrol (3,4',5-trihydroxystilbene) is a phytochemical molecule with clinical/nutraceutical benefits such as anti-inflammatory and anti-oxidative effects. Despite these merits, resveratrol has the following pharmacokinetic drawbacks: (1) limited hydrosolubility lowering efficacy; (2) low chemostability against external environment changes. We resolved the hydrosolubility and chemostability issue of resveratrol by forming resveratrol-β-lactoglobulin complexes, employing Fe(III)-TA nanofilm as a counterpart nanolayer for layer-by-layer (LbL) assembly. The proteinaceous composite nanocoating can be formed in planar and particulate substrates, showing excellent film stability under diverse pH and against digestive enzymes during a weeklong incubation. We envision that the proteinaceous nanocoating herein not only contributes the development of resveratrol delivery systems, but also sheds a light on nanoencapsulation technique carrying diverse hydrophobic cargo materials, such as drugs, nutraceuticals, and micronutrients, for future therapeutic applications.

Poster Presentation : **POLY.P-31**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Light-Mediated Fabrication of Ionogel via Radical Based Thiol-Ene Click Reaction

Jiyeong Yeo, Myungwoong Kim[1,*]

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

Ionogels are the polymer network swollen with an ionic liquid, exhibiting outstanding physical and electrical properties useful for a range of electronic and healthcare applications. Typically, the gels are fabricated through the formation of network by noncovalent interactions. Covalently formed ionogels having potential stability have also been shown with specific reactions such as urethane bond formation. In another perspective, light-mediated formation of the polymer network in ionic liquid enables effective fabrication of the ionogel in desired regions, i.e. the photopatterning. Herein, we demonstrate the photo-crosslinkable ion gel films using thiol-ene click reaction. Thiol-containing multi-arm poly(ethylene oxide) which preferably interacts with ionic liquid molecules was subjected to the crosslinking reaction with properly designed and synthesized methacrylate-containing multifunctional crosslinker and photo-radical generator in ionic liquid and organic solvent. The reaction took place upon the illumination of UV light, yielding well-defined ionogel. The process was further extended to the photopatterning on electronically relevant surface to elucidate the applicability of the process and materials in actual electronic applications.

Poster Presentation : **POLY.P-32**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Photopatternable polymeric systems with controlled surface properties to understand the selective physical vapor deposition of an inorganic material

ChangJae Lee, Myungwoong Kim*

Department of Chemistry, Inha University, Korea

Organic photopatterns on inorganic surfaces provide the versatile route enabling selective physical vapor deposition of functional inorganic materials, e.g. PbI2, which is precursor to synthesize perovskite materials. Ultimately, photolithographically defined organic templates allow the patterning of perovskite in thin film. Herein, for elucidating the surface property-selectivity relationship, photopatternable copolymer systems with systematically varied surface energy were designed and realized. Furthermore, the created organic surfaces were studied using contact angle measurements for surface properties, X-ray photoelectron spectroscopy for surface compositions, and atomic force microscope for surface roughness. The copolymer patterns were subjected to the deposition of PbI2 at different temperatures to investigate the selectivity of the deposition. The effective control of the surface energy difference between the organic pattern and silicon oxide reveals that the the selectivity is attributed to the surface energy difference between the organic surface and the inorganic surface.

Poster Presentation : **POLY.P-33**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Stabilization of the Oil/Water Interface by Amphiphilic Miktoarm Core Cross-Linked polymers

Yunji Jung, Myungeun Seo*

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

Well-Defined miktoarm core cross-linked (CCS) polymers can stabilize an immiscible liquid/liquid interface by letting chemically distinct arms partition into the corresponding liquid phases. The densely cross-linked core, tying the arms together covalently, sits at the interface and provides high adsorption energy. We have developed a facile synthetic strategy to amphiphilic miktoarm CCS polymers that possess many adjustable arms and behave as Janus hairy nanoparticles. Compared to a linear diblock analogue, superior interfacial activities for stabilizing the oil/water interface in a wider composition window and longer stability suggests potential of the CCS architecture for interfacial applications.

Poster Presentation : **POLY.P-34**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Substrate Independent Photoimageable Polymeric Systems with Chemical Versatility Allowing Post-patterning Modifications

Seung Yeon Choi, Sol An[1], Myungwoong Kim[1,*]

Chemistry and Chemical Engineering, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

Protein microarray technology has emerged as a vital bioanalytical tool, which is based on selective immobilization of biological objects. To define site-specifically bioactive films on processable substrates, it is relevant to have substrate independency, patternability, functionalizable surface moiety, and biocompatible surface. Here, we demonstrate substrate-independent photo-crosslinkable copolymer thin films with variable functionalities on film surfaces. The system was achieved with the copolymers synthesized with protic solvent soluble monomer, light-activated monomer, and reactive monomers and therefore, the thin film formation and development upon the light illumination were effectively performed on silicon and polystyrene substrates with protic solvents. The formation of line/space and square patterns were successfully conducted with the systems. The created surfaces were further studied to define different chemical functionalities with the remaining reactive groups upon the photopatterning process, highlighting the potential of our carefully designed and realized photopatterning materials to create functional patterns on a variety of substrates.

Poster Presentation : **POLY.P-35**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Poly(HEMA) Grafting on Plastic Substrates with Low Chemical Reactivity and their Antibacterial Effects

Sang jeong Park, Woo Kyung Cho[1,*]

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

The fouling phenomenon such as non-specific adsorption of proteins and cells onto medical catheter tubes and stents can not only cause the deterioration of the medical tools/devices but also can sometimes be life-threatening. Therefore, the materials used for medical devices should have antibacterial properties, and medical device that are in contact with blood must be hemocompatible. While the functional coatings to suppress fouling have been widely investigated for inorganic substrates such as silicon, gold, titanium, and stainless steel, the study on surface modification for plastic/polymeric substrates due to their low chemistry reactivity. To address this issue, we aimed to develop efficient antifouling coatings for plastic substrates. Poly(methyl methacrylate) and polystyrene were used in this study. The substrates were modified with aryl azide-based photoinitiator via photochemical reaction and functionalized by grafting of poly(hydroxyethyl methacrylate) (poly(HEMA)).The successful surface modification was confirmed by water contact angle goniometry and X-ray photoelectron spectroscopy. To evaluate antifouling capability of the poly(HEMA) coatings, we conducted bacterial adhesion tests using *E. coli.* Compared to controls, the poly(HEMA)-coated substrates could greatly suppress bacterial adhesion.

Poster Presentation : **POLY.P-36**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Aryl Azide-Based, Photochemical Reaction and Surface Zwitteration on Polymeric Substrates for Non-Biofouling Applications

Hyun Ji Seo, Woo Kyung Cho*

Department of Chemistry, Chungnam National University, Korea

Proteins and bacteria can non-specifically adhere to surface of medical devices/tools, which are inserted into the body such as catheters and vascular stents, can cause medical infections and mortality if the case is severe. Many medical devices/tools are made of polymeric materials that are challenging to functionalize due to low chemical reactivity. In this study, we aimed to develop highly effective non-biofouling coatings for polymeric materials including poly(dimethylsiloxane), polystyrene, and poly(methyl methacrylate). Aryl azide-based photoinitiator was synthesized and immobilized onto the polymeric substrates *via* photoreaction and zwitterionic poly(sufobetaine) (poly(SB)) was grafted from the surfaces by oxygen-tolerant atom transfer radical polymerization. The successful chemical modification was confirmed by contact angle goniometry and X-ray photoelectron spectroscopy. Water contact angles significantly decreased after grafting of the poly(SB), compared to control substrates, demonstrating that strong hydration layer can form onto the poly(SB)-coated surface. Non-biofouling capability of the poly(SB) coating was confirmed by antibacterial and antiplatelet experiments. Compared with controls, the poly(SB)-coated substrates could inhibit the bacterial adhesion and also suppress platelet adhesion/activation, showing the excellent non-biofouling effects.

Poster Presentation : **POLY.P-37**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis of Poly[(1,1-dialkyl-3,4-diphenyl-2,5-silolene)-co-(ethynylene)] by the Stille Coupling Reaction of 2,5-Dibromosiloles with Bis(tributylstannyl)acetylene

Ji hun Lee, Young Tae Park[*], Se Yeon Park[1], Hyeong Rok Si[1]

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

Dialkyl(R = Et, or *iso*-Pr, or *n*-Hex)-bis(phenylethynyl)-silanes were reacted with lithium naphthalenide, anhydrous zinc chloride, and *N*-bromosuccinimide (NBS) to obtain 1,1-dialkyl(R = Et, or *iso*-Pr, or *n*-Hex)-2,5-dibromo-3,4-diphenyl-siloles, respectively. Poly[(1,1-dialkyl-3,4-diphenyl-2,5-silolene)-co-(ethynylene)], conjugated polymers containing with silolene and acetylene, were synthesized through the Stille coupling reaction of 1,1-dialkyl-2,5-dibromo-3,4-diphenyl-siloles and bis(tributylstannyl)acetylene as co-monomers, in the presence of toluene as solvent and dichlorobis(triphenylphosphine)palladium as catalyst. The crude products were purified by precipitation with methanol and then furthermore purified by extraction with chloroform. The obtained polymeric materials were analyzed by ^{1}H, ^{13}C, ^{29}Si NMR, FT-IR, GPC and UV-vis spectroscopy.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-38**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Fabricating Pure Polyvinylidene Fluoride with High β-phase Using Thermal Decomposable Additive

Jinwoo Choi, Youngjong Kang[1,*]

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

The beta-phase formed PVDF is well-known for its excellent ferroelectric, piezoelectric, and pyroelectric properties. In this work, the beta-phase structure of PVDF film and fiber is enhanced by adding Butadiene Sulfone. The samples are fabricated by using solution casting, spin coating, and wet spinning with incorporation of varying butadiene sulfone fractions. After fabrication, residue of the butadiene sulfone can be eliminated with vacuum oven. X-Ray diffraction, GI-WAXS and FT-IR are used to study the crystalline nanostructure of PVDF sample. The surface of the polymer is measured through scanning electron microscope(SEM). The measurement about its electroactive property is carried out to compare general PVDF sample with the butadiene sulfone added PVDF sample

Poster Presentation : **POLY.P-39**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Synthesis and characterization of liquid crystal epoxy thermosetting polymer based on phenyl benzoate

Arinola Isa Olamilekan, Hyeonuk Yeo[1,*]

Department of Science Education, Kyungpook National University, Korea

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

Liquid crystal epoxy resins (LCERs) thermoset with high rigidity of mesogenic units in their backbone is expected to form a regular microstructure during curing process and this could enhance it thermal conductivity. Here, a series of twin liquid crystal epoxy resins (LCERs) thermoset based on the phenyl benzoate mesogenic group was synthesised and structurally characterised by nuclear magnetic resonance (NMR) spectroscopy. The mesophase behaviour of the LC monomer was measured by differential scanning calorimetry (DSC) and polarised optical microscopy (POM), the monomer exhibited stable nematic phase at LC temperature range of (115 - 210 °C). 4,4′-diaminodiphenylmethane (DDM) was selected as curing agent base on the LC temperature range, and DSC was used to investigate the curing reaction. The molecular interaction enhanced the thermal conductivity and it showed 0.45 W/mK which is obvious higher than convention ER 0.20 W/mK, the cured sample exhibited a regular microstructure as revealed by XRD measurement and DFT calculation. Also, the cured sample exhibited high thermal decomposition temperature and of ~350 °C and glass transition temperature (Tg) ~100 °C.

Poster Presentation : **POLY.P-40**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis of sequence defined polymer using passerine 3-component reaction

SooJeong Lee, Kyoung Taek Kim[1,*]

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

The synthesis of sequence-defined polymer is an important due to the possibility for developing materials with tunable functions and properties. In the previous studies, the various researches on synthesizing discrete polymers with defined sequences have been conducted. In this study, the sequence-defined polymer is synthesized more efficiently via 3-component passerini reaction. The passerini reaction is a chemical reaction involving an isocyanide, an aldehyde and a carboxylic acid. A polymer with a defined sequence was synthesized by adding a monomer containing a isocyanide group. As a result, the synthesized polymer becomes a material having various functions and physical properties by containing functional groups or side chains at desired location.

Poster Presentation : **POLY.P-41**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Controlling micropore size in hyper-cross-linked polymer via in-situ removal of porogenic templates

Wonjune Yeo, Myungeun Seo[1,*]

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Porous polymers have received a lot of attention due to their diverse pore characteristics such as high surface area, pore size, and pore functionality etc. Hyper-cross-linking of aromatic compounds has been extensively investigated as a synthetically feasible and practical means to producing microporous polymers possessing < 2 nm pores with high thermal/chemical stability. However, control of micropore size has been challenging in the amorphous hyper-cross-linked network despite the huge demand for size-selective separation. Herein, we introduce a new method that allows us to tune the size of micropores produced by hyper-cross-linking at sub-nm level. We will show that a molecular porogenic group that is removed in situ during the hyper-cross-linking reaction templates the micropore size. Synthetic details and characterization will be discussed.

Poster Presentation : **POLY.P-42**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

one-pot synthetic route for simple cellulose nanocrystal functionalization

Bon-Jun Ku, Chiyoung Park[1,*]

Energy Engineering Science, DGIST, Korea
[1]*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Surfaces capable of high-affinity binding of biomolecules are required for many biotechnology applications such as purification, transfection and sensing. Therein, high surface colloidal cellulose nanocrystals (CNCs) are attractive because of their available for functionalization. An intrinsically anionic surface must be cationized in order to take advantage of electrostatic bonding since biological supramolecules are primarily anionic. Our reaction simultaneously leads to nanoization and cationic functionalization of cellulose. The surface substitution rate for the resulting cellulose nanocrystals was verified through XPS, zeta potential and dye adsorption analysis. Also, SEM and hydrodynamic analysis were used to measure size of crystals. This simple process uses very little organic solvents, and the ionic liquids are reusable. Therefore, it is expected to be used as an economical and eco-friendly, meaningful reaction pathway.

Poster Presentation : **POLY.P-43**

Polymer Chemistry

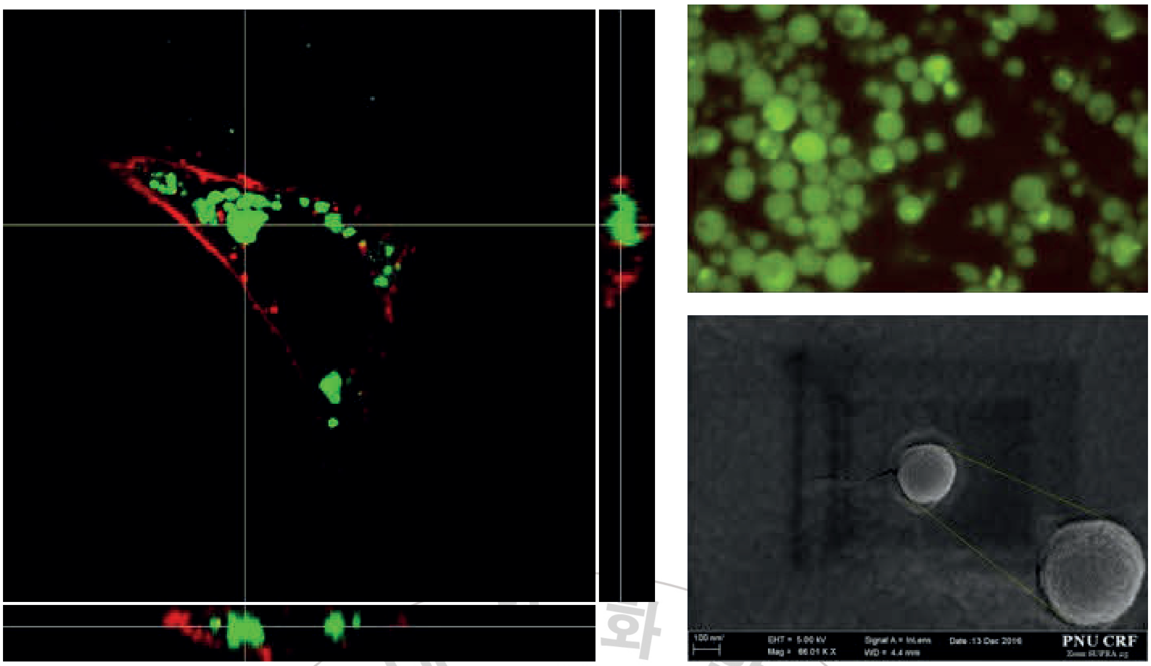
Exhibition Hall 1 THU 11:00~12:30

Biodegradable and biocompatible polyurethanes nanoparticles as drug and DNA gene carriers

Soo-Yong Park, Ildoo Chung[1,*]

Department of Polymer Science Engineering, Pusan National University, Korea
[1]*Department of Polymer Science and Engineering, Pusan National University, Korea*

Gene carrier nanoparticles with minimal toxicity and high transfection efficiency were fabricated from biodegradable polymer (L-tyrosine polyurethane, LTU). In order to evaluate cellular uptake and transfection studies, we prepared fluorescently labeled bovine serum albumin (FITC-BSA) to investigate cellular uptake and pDNA-linear polyethylenimine (LPEI) complex to investigate the transfection efficiency in LX2, HepG2, MCF7 cells. And the second study was progressed with biodegradable polyfumarateurethane (PFU) for use as a bupivacaine delivery vehicle, synthesized using di-(2-hydroxypropyl fumarate) (DHPF), polyethylene glycol (PEG) and 1,6-hexamethylene diisocyanate (HMDI), was designed to be degradable through the hydrolysis and enzymatic degradation of the ester bonds in its polymer backbone. Using double emulsion techniques, LTU and PFU nanoparticles were fabricated encapsulating drug or gene, to avoid the immune system their surface was modified with PEG.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PNU CRF
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Poster Presentation : **POLY.P-44**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

[Withdrawal] Crystallization-Driven Self-Assembly of Block Copolymers having Monodisperse Poly(lactic acid)s with Defined Stereochemical Sequences

Kyoung Taek Kim*, Yongbeom Kwon

Division of Chemistry, Seoul National University, Korea

Poster Presentation : **POLY.P-45**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Mussel-Inspired Zwitterionic Copolyethers with Antifouling Effect

MinJung Kim, Byeong-Su Kim*

Department of Chemistry, Yonsei University, Korea

With their superior hydrophilicity, zwitterionic molecules are known to form a strong hydration layer serving as an effective antifouling material. Despite their widespread use, the immobilization of zwitterionic molecules on various surfaces has posed a considerable challenge. Herein, we design the zwitterionic polyethers functionalized with mussel-inspired catechol moiety for versatile surface coating with high antifouling property. A series of block polyethers were synthesized via sequential anionic ring-opening polymerization of catechol-acetonide glycidyl ether and *N,N*-diisopropyl ethanolamine glycidyl ether, followed by post-polymerization modification to afford the desired zwitterionic brushes. Successful polymerization was confirmed using ^{1}H, ^{13}C-NMR, GPC, FT-IR and DSC measurements. The versatile surface adsorption and superior antifouling effects of synthesized polyethers were evaluated using atomic force microscopy (AFM) and quartz crystal microbalance with dissipation (QCM-D). This study demonstrates that bifunctional polyether bearing long zwitterionic chain shows superior antifouling effect, presenting its prospective applications in various fields.

Poster Presentation : **POLY.P-46**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Mechanochemical Fabrication of Vitrimer-CNT Composites for Highly Sensitive Temperature-Resistance Sensor

Wansu Cho, Chiyoung Park*

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

Carbon nanotube (CNT) is one of the most well-known conducting carbon materials which can provide electrical and enhance mechanical property to polymer binders. Despite of these advantages, difficulty of well dispersing CNTs due to bundling caused by van der Waals interaction between tube surfaces makes it hard to applicate CNTs instantly. General ultrasonication assisted exfoliation in organic solvents requires long time process and multi-steps to fabricate polymer-CNT composites. Here, we suggest quick mechanical fabrication of vitrimer-CNT composites through simple grinding with an aromatic molecule and demonstrate its highly sensitive temperature-resistance sensing properties.

Poster Presentation : **POLY.P-47**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

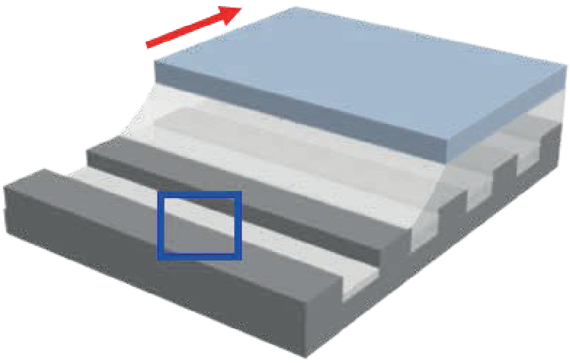
Generation of 2D DNA microstructure under topographic template and shear force

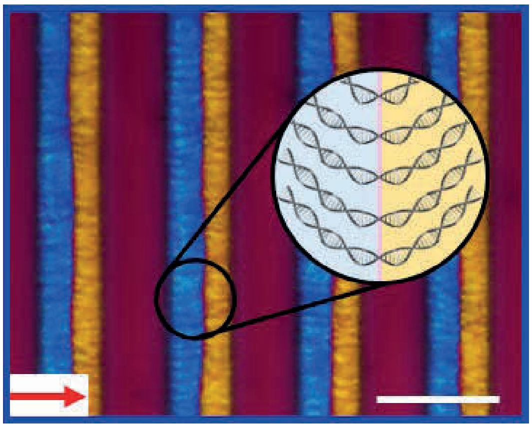
Soon Mo Park, Dong Ki Yoon[1,*]

Graduate School of Nanoscience and Technology, Korea Advanced Institute of Science and Technology, Korea

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

Deoxyribonucleic acid (DNA) has recently emerged as one of the promising building blocks because it is abundant in nature, shows lyotropic liquid crystal (LC) phase, and can be easily functionalized with additives through electrostatic interaction. Controlling the order and orientation of DNA chains is quite difficult due to the long contour length and flexibility but is necessary for forming the micro- or nanostructures to utilize as practical applications. Therefore, we developed a technique to control the order and orientation of DNA chains in a thin film by using shear-induced pre-alignment and anisotropic elasticity of the DNA LC phase. Predesigned substrates were applied to give confinement effect which determines the final director configuration of this soft material. Then, complicated two-dimensional micro- or nanostructures could be formed spontaneously due to the interaction between the elastic properties of DNA and the confinement effect of the substrate.





Poster Presentation : **POLY.P-48**

Polymer Chemistry

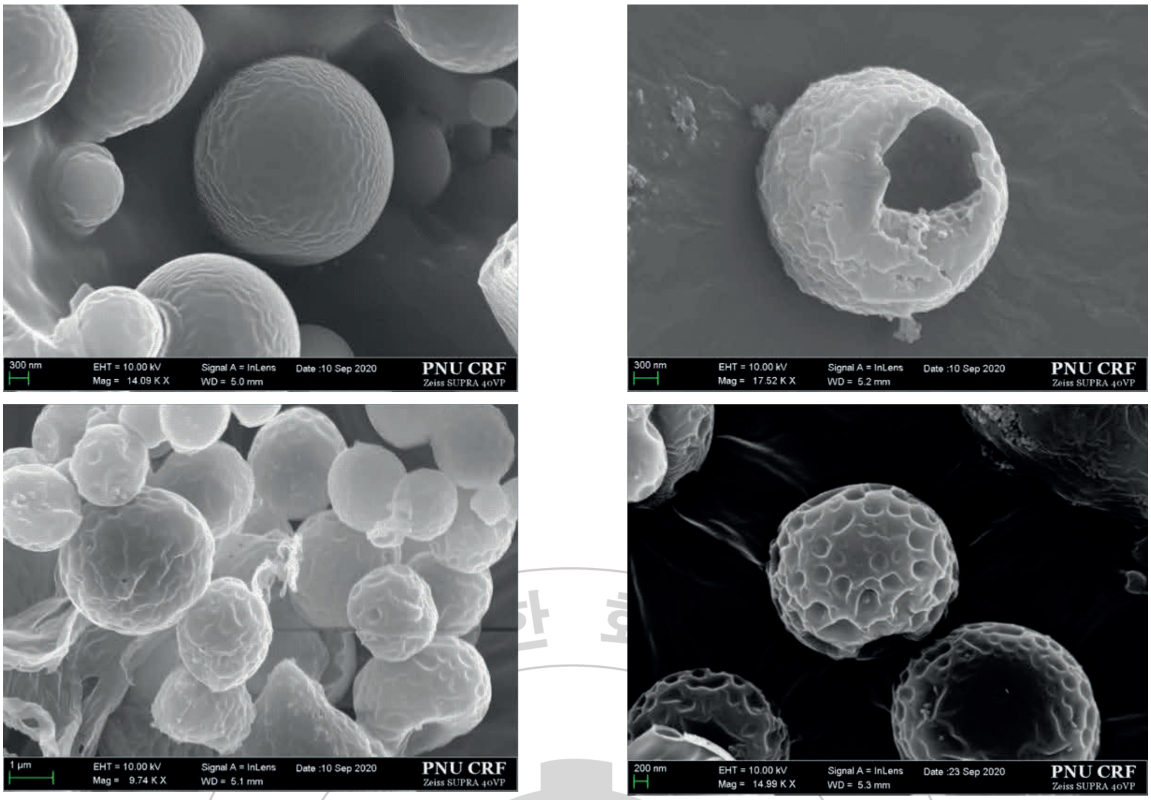
Exhibition Hall 1 THU 11:00~12:30

Synthesis and characterization of thermoresponsive hollow polymeric shell particles based on colloidal silica

Soo-Yong Park, Ildoo Chung[*]

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

In this study, PNIPAAm-grafted thermoresponsive hollow-polymeric-shell (HPS) particles with a connecting holes the outside were prepared from surface-modified colloidal silica (CS) with poly(ethylene glycol) methyl ether-3-(triethoxysilyl)propyl isocyanate (PEGME-IPTES) as templates. Colloidal silica nanoparticles were synthesized using tetraethoxysilane (TEOS) and distilled water in methanol with ammonia solution (NH_3) as a catalyst by the sol-gel method. PEGME-IPTES was synthesized using a 3-(triethoxysilyl) propyl isocyanate (IPTES) with poly(ethylene glycol) methyl ether (PEGME) in the presence of dibutyltin dilaurate and characterized by ^{1}H NMR, ^{13}C NMR, FT-IR spectroscopies. The PNIPAAm-grafted CS particles were prepared by modified silica with 3-(trimethoxysilyl) propyl methacrylate (MPS) and PEGME-IPTES by the polymerization of poly(N-isopropylacrylamide) (PNIPAAm), then the modified silica core with PEGME-IPTES on the surface were removed by etching with hydrofluoric acid. The chemical characterization of bare CS, modified CS, PNIPAAm, PNIPAAm-CS, HPS particles was characterized by FT-IR spectroscopy. In order to confirm the LCST property of the HPS particles , the transition of transmittance and the change of particle diameter according to the temperature change were measured through UV-vis spectroscopy, DLS and microscope. In addition, the size and shape of the HPS particles were determined by TEM and SEM.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Date :10 Sep 2020
PNU CRF
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PNU CRF
Zeiss SUPRA 40VP

Poster Presentation : **POLY.P-49**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Enhanced catalytic glycolysis conditions for chemical recycling of glycol-modified poly(ethylene terephthalate)

Minh Dieu Ngo, Kyuwon Sim[1], Hyun Min Jung[1,*]

Department of Applied chemistry, Kumoh National Institute of Technology, Korea
[1]*Department of Applied Chemistry, Kumoh National Institute of Technology, Korea*

Recently, poly (ethylene terephthalate) (PET) and its glycol-modified derivatives, such as poly (1,4-cyclohexylenedimethylene terephthalate) (PCT), poly (isosorbide terephthalate) (PIT) have been used widely due to their good thermal and mechanical properties. Besides, the demand for their chemical recycling is also rising. However, systematic studies on the glycolysis activity of PET derivatives have been limited. In our study, glycolysis of PET with diethylene glycol (DEG), 1,4-cyclohexanedimethanol (CHDM) and D-isosorbide (ISB) under catalytic conditions was investigated. ISB and CHDM showed low reactivity due to its unreactive structure. It was founded that the increased nucleophilicity of the alkoxide-combined zinc catalyst improved the reactivity of transesterification. The enhanced catalytic glycolysis condition was applied to the glycolysis of PCT; the reaction rate was three times higher than that with the conventional zinc acetate and the product was produced with 82% yield.

Poster Presentation : **POLY.P-50**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Hydrogel-coated lateral flow strip platform for the rapid COVID-19 detection

Kwanwoo Shin[*], Nayoon Pyun[1], Eunjin Huh[1]

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

Point-of-care (POC) devices that enable rapid point-of-care diagnosis are of great importance in environments with poor medical conditions or infectious diseases, which have recently become a big problem worldwide. Among the various POCs, paper-based cross-flow strips using capillary and serological analysis methods have attracted much attention due to their ease of use and economical aspects. However, this method also has drawbacks. They often show relatively low sensitivity. The substrate for these strips is made primarily of cellulose, which lacks binding sites for biomolecules that can detect analytes for proteins with chemically inert properties, especially high hydrophobicity. Additionally, these strips can be difficult to control flow, which affects sensitivity.In this research, a lateral-flow strip sensor was developed to detect the antibody of SARS-CoV-2 by using hydrogel instead of paper to increase the sensitivity. To improve protein adsorption on the substrate, a hydrogel made by adding polystyrene nanoparticles to a hydrophilic PEGDA hydrogel precursor was used. This can lower the background and also enhance the binding capacity with controlled hydrophilicity. We confirmed that the sensitivity can be also improved by adjusting the flow rate of the analyte sample through the hydrogel-coated strip. In this presentation, we will introduce 1) the design of the hydrogel-based lateral flow chip developed and 2) the experimental results on the COVID responses using this chip.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **POLY.P-51**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Effective Synthesis of Polymer Catenanes Composed of Interlocked Discrete Cyclic Polymers

Mo Beom Koo, Junyoung Kim[1], Kyoung Taek Kim[2,*]

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

Cyclic polymers have attracted scientific and practical attention due to their unique set of properties arising from the restricted chain conformation and the lack of end groups. The synthesis of discrete cyclic polymers and block copolymers was recently reported using the combination of the iterative convergent method and the intramolecular cyclization. The studies on cyclic polymers without trace amounts of linear contaminants were performed to provide fundamental insights into the chemical and physical properties. In addition, polymer catenanes, composed of interlocked cyclic polymers, were prepared by the template threading approach. Using the linear convergent method, functional monomers were precisely placed into polymer chains to make use of intermolecular interactions as a binding force. The binding interactions induced a linear chain to thread through cyclic polymer, leading to the efficient preparation of polymer catenanes.

Poster Presentation : **POLY.P-52**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Lyotropic Bilayer-folded lamellar mesophase in an amphiphilic random copolymer hydrogel

Minjoong Shin, Myungeun Seo[1,*]

Graduate School of Nano Science Technology, Korea Advanced Institute of Science and Technology, Korea

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

Amphiphilic copolymers which contain repeating hydrophilic and hydrophobic pendant groups randomly self-assemble into spherical micelle in an aqueous solution driven by hydrophobic interaction. At higher concentrations, an anisotropic, birefringent hydrogel phase emerges based on the lamellar packing of micellar bilayers. Here we report the lyotropic phase behavior of their aqueous solutions in concentrated regimes. In x-ray scattering investigations, a phase window forming a physical gel is discovered, with a structural hierarchy ranging from sub-20 nanometers to several angstroms. Under shear, the mesophase could be conveniently oriented to demonstrate anisotropy.

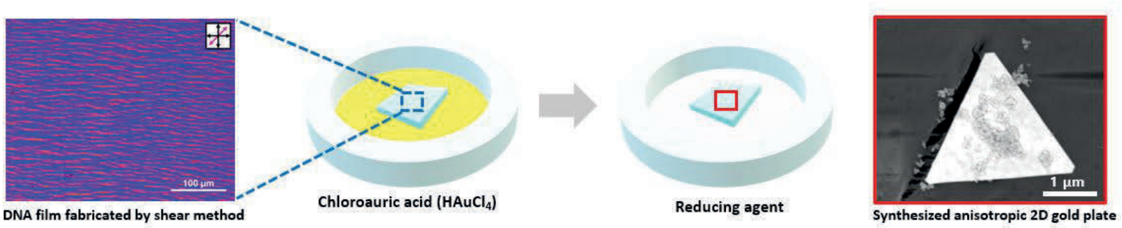
Poster Presentation : **POLY.P-53**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Nucleation and Growth of Two-dimensional Gold Plates on DNA Film

Juri Kim, Dong Ki Yoon*

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

Nano- and micro-sized metal plates have recently been interested in promising functional building blocks due to their high surface-to-volume ratio, unique optical & electrical properties. However, synthesis of anisotropic 2D metal particles require elaborate multi steps such as shape transformation by etching process or seeded growth process. Therefore, we developed a method to synthesize 2D inorganic particles by using DNA film as a template. It is well known that DNA shows liquid crystal phase depending on the concentration. Oriented DNA film can be formed by simple coating process inducing competitive interaction between shearing force and elastic energy minimization during water evaporation. Since this film has a dense negative charge on the surface, it can be used as a template for synthesizing various inorganic particles by forming charge complex with metal ions. Here, we synthesized anisotropic two-dimensional gold particles by simply dipping preformed DNA film into chloroauric acid solution and reducing agent sequentially. Nano- and micro-sized particles have been successfully synthesized, and order & orientation of DNA chains in the film are maintained even after all procedures. This will offer possibility of other biomaterials, including DNA, as a versatile platform for nucleation and growth of inorganic compounds.



Poster Presentation : **POLY.P-54**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Morphological stability of Cross-linkable polymers in organic solar cells

Minhun Jee, Ziang Wu, Han Young Woo*

Department of Chemistry, Korea University, Korea

The power conversion efficiencies (PCE) of the donor polymer and small molecular acceptor blend system are high, but the stability against heat and light is poor. The heat generated by light increases the free volume due to the long-range segmental motion of molecules in the active layer, allowing oxygen and moisture to penetrate the device. In addition, it shows the change in the morphology of the bulk heterojunction (BHJ) device due to diffusion and aggregation of the small molecular acceptor. An increase in domain size and phase separation is induced. As a result, the stability to heat is decreased and the performance as a solar cell device has deteriorated. The introduction of cross-linkable functional groups can lead to morphological stability. Our research group synthesized PM6-Br having an appropriate amount of Br that can be crosslinked and tested the device with Y6. As a result, we get the high efficiency, but the thermal stability was not significantly different from that of the existing PM6:Y6. Choi et al research stability in organic solar cells with cross-linkable donor and acceptor. Both electron donor and electron acceptor show high thermal stability(91%) for 90min when cross-linkable functional groups are introduced (PBDBT BV20:N2200-TV10). Recently, papers showing high efficiency while having an appropriate molecular weight when Y5 material is made into a polymer have been published. We are synthesizing a Y5-based cross-linkable electron acceptor. Since PM6-Br, which can be crosslinked with high efficiency, has already been obtained, it is expected devices with high efficiency and stability.

Poster Presentation : **POLY.P-55**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis and Characterization of New Organic Semiconductor ITIC Acceptor

Ji Eun Lee, Yun Hi Kim[1,*]

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

A acceptor materials are designed and synthesized for organic solar cells(OSCs). We developed efficient fused-ring electronic acceptors based on indacenodithieno[3,2-b]thiophene(IT) core and 2-(alkylthio)thienyl side chains. We developed alkylthiothienyl side chains instead of thienyl side chains in order to get lower HOMO levels and highter electron mobility.The properties and structure of synthesized acceptor materials were characterized by H-NMR. The thermal characteristics of the fabricated material were measured by DSC and TGA.

Poster Presentation : **POLY.P-56**

Polymer Chemistry

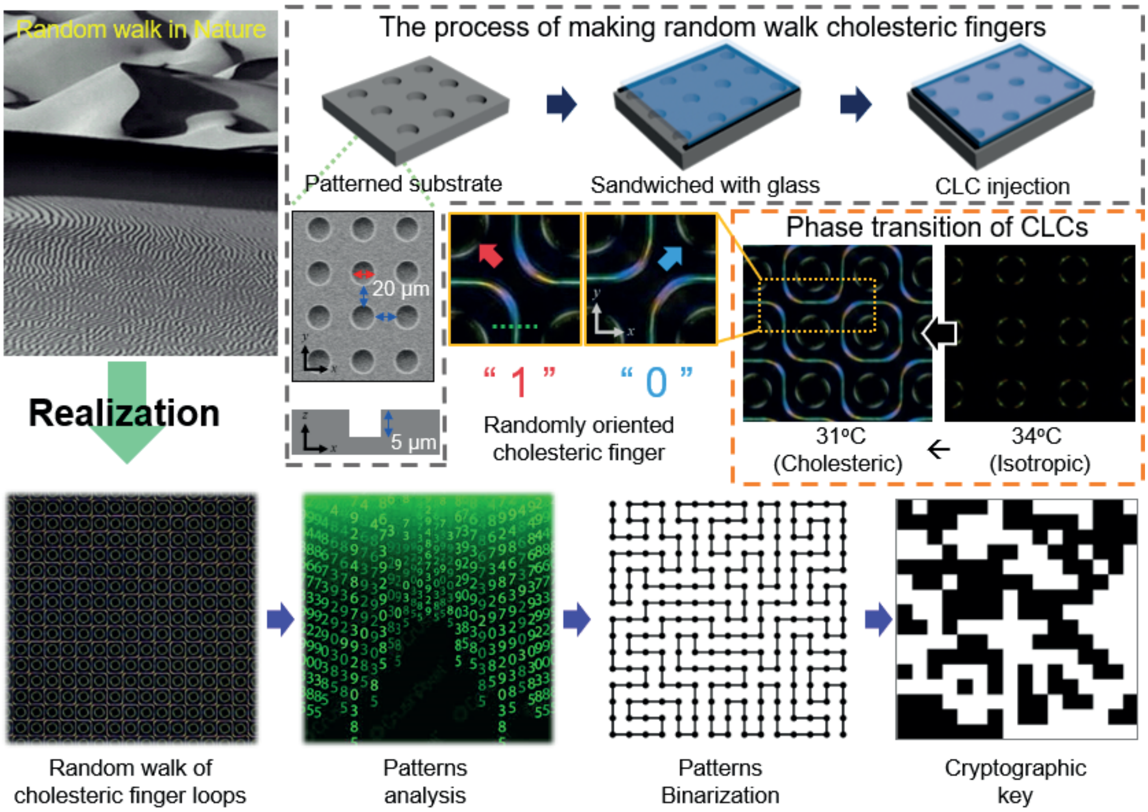
Exhibition Hall 1 THU 11:00~12:30

Fabrication of Physical Unclonable Function with self-assembled chiral liquid crystals via defect engineering

Dong Ki Yoon[*], Geonhyeong Park[1]

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

Defects are regarded as entities that have to be removed for better performance in most of materials. However, in recent years, interests in controlling the defect structures itself of liquid crystals are increasing due to their unique properties. Defect engineering with liquid crystals have been applied to various scaffold for lithography, soft actuators, controlling living matter, and scaffold for self-assembly. The defects of the liquid crystals have various structures such as point, ring, and line according to the molecular arrangement around the defect cores. Here, we fabricated the complex defects arrays by using the appropriate confinement effect and the intrinsic elasticity of the liquid crystal. These defects act as seeds for the assembly of chiral liquid crystals and assemble them in a random pattern with a lattice. These assembled patterns memorize the randomness or natures because their formation is governed by thermal fluctuations. We showed that these arbitrary patterns can be applied on a physical unclonable function (PUF), similar to artificial fingerprints, by using object detector based on deep learning. In addition, they have reconfigurability that is not possible with silicon-based PUF because this self-assembly is fully. This new authentication tag based on self-assembly is expected to be able to prevent attacks on personal information effectively in the coming 4th industrial revolution era.


Random walk in Nature
The process of making random walk cholesteric fingers
Patterned substrate
Sandwiched with glass
CLC injection
20 μm
5 μm
y
x
z
"1"
"0"
Randomly oriented cholesteric finger
Phase transition of CLCs
31°C (Cholesteric)
34°C (Isotropic)
Realization
Random walk of cholesteric finger loops
Patterns analysis
Patterns Binarization
Cryptographic key

Poster Presentation : **POLY.P-57**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Homojunction Field-Effect Transistors with selectively doped conductive polymer electrode

Yoonjoo Lee, Han Young Woo[1,*]

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

The research on conductive polymer electrodes has attracted great attention due to the increasing demand for completely foldable electronics that are mechanically robust. However, weak physical adhesion at intrinsic heterojunctions has limited its applicability in foldable devices. Herein, selectively-doped p-type diketopyrrolopyrrole (DPP)-based semiconducting polymer films wirh $FeCl_3$ were used as source/drain electrodes in homojunction-based polymer thin-film transistors (PTFTs). The gradual work function change with depth was generated via sequential doping process, which reduced energy barrier between electrode and semiconducting region, consequently having low contact resistance and promoting charge injection. In addition, mechanical stbility at interfacial adhesion in PTFTs was enhanced by interfacial crosslinking at heterojunction. The electrical performance of resulting PTFTs showed great stability even after extreme folding, proving that the proposed device fabrication strategy is promising for various completely foldable electronics.

Poster Presentation : **POLY.P-58**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Development of Boron-Based Efficient and Pure Blue TADF Materials for Organic Light Emitting Diodes

Hyung Jin Cheon, Kim Jang-Joo[1], Soon-Ki Kwon[2], Yun Hi Kim[*]

Chemistry, Gyeongsang National University, Korea
[1]*Materials Science and Engineering, Seoul National University, Korea*
[2]*Materials Engineering and Convergence Technology, Gyeongsang National University, Korea*

The development of thermally activated delayed fluorescent (TADF) emitters has greatly improved the efficiency of the fluorescent organic-light emitting diodes (OLEDs). New highly efficient thermally activated delayed fluorescence (TADF) dopant materials (TDBA-SAF, DBA-SAB) for blue organic light-emitting diodes are reported. The blue TADF device with TDBA-SAF in the DPEPO host exhibited a maximum EQE of 28.2% with CIE coordinates of (0.142, 0.090).

Poster Presentation : **POLY.P-59**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

How to enhance the thermal stability of block-polymer templated nanoporous polymers

Taeseok Oh, Wonjune Yeo, Myungeun Seo*

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

Block polymer templating offers a fascinating route to well-defined nanoporous membranes with robust pore size control and surface tailorability useful for separators in electrochemical devices. However, fabricating the membranes on a large scale with sufficient thermal stability and mechanical integrity has been challenging and limited their applications. Thermal stability is particularly important to ensure a wide range of operational temperature windows for the target application. Here we investigate thermal stability as a criterion to retain the pore structure at a given temperature without pore collapse. The influence of the polymer framework, the cross-linking density, and the pore size on thermal stability will be discussed.

Poster Presentation : **POLY.P-60**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Templated Synthesis of ordered mesoporous carbons (OMCs) by using polymer cubosomes as templates and their electrochemical applications.

Jeongeun Song, Kyoung Taek Kim*

Division of Chemistry, Seoul National University, Korea

Various mesoporous carbon materials have been studied for applications in the field of energy conversion, energy storage, separation, and catalysts. They have the potential to be used as an electrode material for electrochemical capacitors due to their high surface area and physical and chemical property. Many mesoporous carbon materials were synthesized through replication from porous materials used as molds. Polymer cubosomes (PCs) are a new polymeric mesoporous material that contains two non-intersecting water-channel networks with the internal crystalline order. We obtained new ordered mesoporous carbon (OMC) particles via templated synthesis using PCs as templates and furfuryl alcohol as carbon precursors. The water-channel networks of PCs were translated into carbonaceous skeletal networks as furfuryl alcohol was polymerized inside the water-channel networks under acidic conditions without collapse of the internal structure of PCs as templates. The interconnected networks of the resulting OMC particles improve the molecule diffusion and electrolyte ion transportation because of the increased surface area and the electrochemical conductivity of OMC particles. Thus, OMC particles could be likely to an electrode of supercapacitors and have shown corresponding electrochemical experimental results.

Poster Presentation : **POLY.P-61**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis and drug-eluting behavior of biodegradable hydrogel beads

Jeewon Do, Wonmok Lee[1,*]

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

In this study, various studies were conducted with the aim of producing a drug eluting bead using 3-sulfopropyl methacrylate (SPMA) having a sulfonyl group that can absorb doxorubicin (DOX), an anticancer drug widely used in breast cancer, lung cancer, and liver cancer. Two types of approaches were carried out. First, an opal-templated porous hydrogel of SPMA and (Hydroxyethyl)methacrylate (HEMA) was copolymerized to increase the surface area so that DOX can be absorbed quickly. Secondly, SPMA was copolymerized with Gelatin-methacrylate (GelMA) in a water in oil environment to create bead shaped GelMA hydrogel. GelMA is a chemically modified gelatin with methacrylic anhydride (MA) which has excellent biocompatibility and chemical reactivity. By controlling the SPMA content for each bead, the loading and releasing capabilities of DOX were investigated, and the biodegradability was examined.

Poster Presentation : **POLY.P-62**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Synthesis and Characterization of Orange Phosphorescent Emitting Material

Ji Hyun Lee, Yun Hi Kim*, Hyung Jin Cheon

Department of Chemistry, Gyeongsang National University, Korea

An organic light emitting diode material using phosphorescence can have high luminous efficiency. Because heavy metal complexes such as iridium generate phosphorescence, and this phosphorescence uses both triplet and singlet excitons, the luminous efficiency increases.White OLED using such phosphorescence has advantages in terms of efficiency and lifespan, so it is in the spotlight in the display enlargement and lighting market. WOLED can be implemented in two colors: sky blue and orange. Therefore, there is a need to develop an effective orange material.In this research, we synthesis and design of the new iridium complex as orange phosphorescent emitting material.

Poster Presentation : **POLY.P-63**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Organic phototransistors based on newly synthesized conjugated polymers

Hyunji Son, Chulyeon Lee[1,*], Hwajeong Kim[1,*], Youngkyoo Kim[1,*]

융합학부, Kyungpook National University, Korea
[1]*Department of Chemical Engineering, Kyungpook National University, Korea*

Conjugation polymers are very attractive semiconductor materials for advanced electronic products with their flexible and wearable capabilities compared to inorganic materials. These have been synthesized and applied to organic light-emitting devices, organic solar cells, organic field-effect transistors (OFETs), organic memory devices, etc. through numerous studies due to their potential for flexible electronic devices. A lot of research is currently underway, and especially the longer lengths of the conjugated polymers allow for better charge transport. In this presentation, organic phototransistors (OPRTs) were created by taking advantage of its great flexibility. First, after synthesizing several polymers based on IDTT, organic phototransistors were made and properties were investigated. The next study fabricated and characterized organic phototransistors that detect light from UV (ultraviolet) to NIR (near infrared). These studies have made it possible to demonstrate flexible devices.

Poster Presentation : **POLY.P-64**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Simplified fabrication of EWOD-based chip using PES/PSU thin film

Hyuckjin Lee, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

Electrowetting on a dielectric (EWOD) is useful phenomenon and has been applied in many devices such as displays, optical lens and lab-on-a chip. The fabrication method of EWOD-based chip requires many steps of patterning the conductive electrodes on the substrate and then sequentially processing for coating of the dielectric, hydrophobic and lubricant layers. To simplify these many steps, we employed polyethersulfone (PES) thin film as a dual role of substrate and dielectric layer. For that, we deposited electrodes directly on PES film by using inkjet printing and then flipped it, so that the PES film takes a role a dielectric layer. PES thin film has advantages of flexible, thermostable, transparent, low-cost, simple to fabricate film and suitable for printing. However, fabrication of elaborate film for printing is sensitive to humidity over 30%. When printing on thin film, we require film strength to be easily reproducible without wetting or tearing. After printing, the appropriate pore size of the film should be controlled to be conductive between the nanoparticles of the electrode. We're trying to improve these problems by mixing the polysulfone (PSU) with PES. If these conditions are optimized, it will be possible to fabricate EWOD-based chips more simply and cheaper than before, and it is expected that various advantages of thin polymer films will be utilized in wearable devices or electronic displays.Keywords: Electrowetting on a dielectric (EWOD), Lab-on a chip, thin film, polymer, polyethersulfone (PES), polysulfone (PSU), printing, fabrication

Poster Presentation : **POLY.P-65**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Conjugated Polyelectrolytes with Different Counterions as Hole-Transporting Layer for Sky Blue-Emissive Perovskite Light-Emitting Diodes

Amit Kumar Harit, **Han Young Woo**[1,*]

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

Crystal growth and interfacial defect passivation are essential to achieve high performance in perovskite light-emitting diodes (PeLEDs). Here, a series of poly(fluorene-co-phenylene)-based anionic conjugated polyelectrolytes (CPEs) were prepared with varying sizes of counterions (tetramethylammonium, tetraethylammonium, and tetrabutylammonium (TBA^+) and studied as a hole transport layer (HTL) for sky blue-emissive PeLEDs. The hydrophilic ionic functionality and counterions of CPEs enhance the wettability (or compatibility) and facilitate nucleation to form highly crystalline perovskite crystals at interfaces. Besides, bulkier counterion CPE (MPS2-TBA) reduced phonon-electron coupling and enhanced exciton binding energy more efficiently than widely used HTL PEDOT:PSS in perovskites. Through space charge limited current measurements, the lowest trap density is measured in the perovskite film on MPS2-TBA, emphasizing a critical role of larger counterions. By density functional theory, MPS2-TBA is calculated to show the strongest adsorption affinity toward the interstitial defect of lead ions, explaining its pronounced interfacial defect passivation. Finally, the sky blue-emissive quasi-2D PeLED with MPS2-TBA shows the highest luminance efficiency (a peak EQE of 2.6% at 489 nm) and significantly improved spectral stability.

Poster Presentation : **POLY.P-66**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Near-Infrared Organic Phototransistors with Conjugated Polymer

Yeonhwa Cho, Chulyeon Lee, Hwajeong Kim, Youngkyoo Kim*

Department of Chemical Engineering, Kyungpook National University, Korea

Organic phototransistors have attracted great attention for the last decade because of their capability as a next-generation photodetector platform in the flexible electronics era. Of various organic materials, conjugated polymers have been recognized one of the best candidates for organic phototransistors when it comes to potential roll-to-roll processes using solutions at room temperature leading to ultrathin and flexible photodetector modules. In particular, organic phototransistors have an advantage of signal amplification and active sensing array compared to typical photodiodes. In fact, ultraviolet and visible light detection by organic phototransistors is relatively easy because most organic materials can absorb light at the ultraviolet and visible ranges. However, a near infrared (NIR) range is a bit challenging to detect because a limited number of conjugated polymers are available for the absorption of NIR light. In this presentation, we demonstrate the influence of film thickness on the performance of NIR light-detecting p-channel organic phototransistors with a sensing channel layer of conjugated polymers containing sulfur and nitrogen atoms and their possibility for light detection and ranging (LiDAR) applications.

Poster Presentation : **POLY.P-67**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis and characterization of superabsorbent polymer using poly(itaconic acid) with high reswelling absorption capacity

Hyesun Choi, Jiwon Lee*

Environment, Health and Welfare Research Center, Korea Institute of Science and Technology, Korea

Superabsorbent polymer (SAP) is a three-dimensional (3D) functional hydrogel that can absorb and retain the liquid more ten to hundred times than its initial weight. Commercial SAPs were typically made of a non-degradable petroleum-based polymer such as poly(acrylic acid), poly(acrylamide), poly(methacrylic acid), and poly(acrylonitrile). However, those are not biodegradable, thus can eventually cause the environmental pollution. In this study, a novel environmental-friendly SAP was synthesized based on itaconic acid(IA) as a monomer. As it is a fermented product produced by fungus, IA has the high potential to replace petroleum-based polymers because it has non-toxic and biodegradable properties. Our present work, the cross-linked poly(itaconic acid) (c-PIA) was synthesized by the radical polymerization, followed by the characterization of c-PIA using FTIR, SEM, and rheometer. The water absorption capacity of c-PIA was evaluated both in water and saline solutions. We found c-PIA had the higher water absorption capacity (~330 g/g in deionized water) as well as reswelling absorption capacity (~1100 g/g in deionized water) under each condition.

Poster Presentation : **POLY.P-68**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Enantiopure ω-Substituted Hydroxyalkanoates from Simple Epoxides and Alkenes as Building Blocks for Sequence-Defined Poly(hydroxyalkanoates)s

DoGyun Kim, Jeong Min Lee, Kyoung Taek Kim[*]

Division of Chemistry, Seoul National University, Korea

Poly(hydroxyalkanote) (PHA) is a class of aliphatic polyesters produced naturally by microbes as an energy and carbon reserve. These bio-derived aliphatic polyesters have attracted recent attention as degradable substitutes for hydrocarbon-based polymers used for plastics and packaging materials. However, the biosynthesis of PHAs having diverse side chains has been difficult due to the limited number of engineered microbes for the diversification of poly(3-hydroxybutyrate) (P3HB). Herein, we report the synthesis of enantiopure ω-substituted HAs using racemic epoxides and alkenes as precursors. Our synthesis allows the substituent of HA to be selected from a variety of alkyl, aryl, and functional groups. The stereochemistry of substituted ω-carbon and the number of carbon atoms of HA can also be defined. The resulting enantiopure HAs serve as building blocks to synthesize monodisperse PHAs with defined sequences and stereoregularities via an iterative convergent pathway. Our results could pave the way to engineer PHAs and related polymers with structural sophistication exhibited only by biopolymers such as proteins and nucleic acids. From arbitrary olefin molecules, chiral hydroxyalkanoate (HA) monomers were obtained in 5–7 steps. Through the selection of the olefin molecule, the side chain and length of the backbone of PHA can be varied. Especially, (S)-allyl 6-bromo-3-((tert-butyldimethylsilyl)oxy)hexanoate, from bromo-1-butene, can act as a versatile handle. Molecularly defined PHAs were synthesized by the iterative linear convergence of orthogonally protected HAs. Characterization of PHAs' molecular structure was performed using mass spectroscopy, size exclusion chromatography (SEC), and NMR spectroscopy.

Poster Presentation : **POLY.P-69**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

NONFULLERENE-FULLERENE HYBRID ACCEPTORS FOR ORGANIC SOLAR CELLS

Ziang Wu, Bumjoon Kim[1,*], Han Young Woo[*]

Department of Chemistry, Korea University, Korea
[1]*Department of Chemical Engineering & Biotechnology, Korea Advanced Institute of Science and Technology, Korea*

Organic solar cell (OSC) is continually attracting people's attention due to its high processability, structure variability, and flexibility. In this work, two fullerene-nonfullerene hybrid acceptors, IDTIC-PC$_{61}$BM (IP) and PC$_{61}$BM-IDTIC-PC$_{61}$BM (PIP), are synthesized by combining a nonfullerene acceptor, 3,9-bis(2-methylene-(3- (1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl) -dithieno [2,3-d:2',3'- d']-s-indaceno[1,2-b:5,6-b']dithiophene (IDTIC), and a fullerene derivative, phenyl-C$_{61}$ butyric acid methyl ester (PC$_{61}$BM). Organic solar cells (OSCs) based on the four different acceptors (i.e., IP, PIP, IDTIC, and PC$_{61}$BM) and the same polymer donor (PBDB-T) were fabricated. In IP and PIP, the IDTIC moiety compensates for the poor light absorption of PC$_{61}$BM in the visible wavelength region, improving the short-circuit current density (J_{SC}) of the hybrid acceptor-based OSCs (11.9 → 13.1 mA cm^{-2}). Meanwhile, the charge transport and recombination properties of the PBDBT: IDTIC devices improve significantly after the substitution of IDTIC with IP or PIP, leading to a significant increase in the fill factor (0.54 → 0.68) as well as J_{SC}(11.8 → 13.1 mA cm^{-2}) of the devices. Therefore, owing to the synergistic effect of the broad light absorption of IDTIC and efficient electron transport of PC$_{61}$BM, the hybrid acceptor-based OSCs show significantly higher power conversion efficiencies of 8.81% (PBDB-T:PIP) and 8.17% (PBDB-T:IP) than the PBDB-T:PC$_{61}$BM(7.62%) and PBDB-T:IDTIC (5.98%) OSCs. The results demonstrate the effectiveness of the hybrid acceptor design in overcoming the shortcomings of individual acceptors and improving their photovoltaic performance.

Poster Presentation : **POLY.P-70**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Impact of Polar Side Chain Engineering of CDT-based p-type polymers on Thermoelectric Devices

Ayushi Tripathi, Han Young Woo*

Department of Chemistry, Korea University, Korea

Driven by the prospects of organic thermoelectric(OTE) devices, which have the potential for energy generation, have gathered considerable attention worldwide. We compared various properties of poly[(4,4'-(bis(hexyldecylsulfanyl)methylene)cyclopenta[2,1-b:3,4-b']dithiophene)-alt (benzo[c][1,2,5]thiadiazole)] (PCPDTSBT) and its analogue with oligoethylene glycol (OEG) side chains in place of alkyl ones (PCPDTSBT-A), before and after doping. Incorporation of polar OEG side chains improves intermolecular ordering and exhibits 'self-doping' with enhancement in doping efficiency, thereafter resulting in higher electrical conductivity and power factor of PCPDTSBT-A surpassing those of PCPDTSBT. OEG chains improve the miscibility of dopant solution and polymer film during sequential doping which was performed by casting dopant solution (by varying the concentration of F4TCNQ in acetonitrile) onto the film. This study emphasizes the importance of the polar side chain engineering to modulate doping efficiency, inter-chain packing, crystalline morphology and miscibility whose outcome is revamped electrical and thermoelectrical properties.

Poster Presentation : **POLY.P-71**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Low bandgap polymer-based near infrared organic photodetectors

WonJo Jeong, In Hwan Jung[1,*]

Department of organic and Nano Engineering, Hanyang University, Korea
[1]*Department of Organic and Nano Engineering, Hanyang University, Korea*

The photoconductivity conjugated polymers PDTPTT and PCPDTTT used DTP and CPDT, which are strong electron donating moieties. It is a system with a fused ring in common, and solubility can be controlled by using an alkyl chain. This could be easily controlled with the fused carbon of the CPDT and the nitrogen of the DTP. DTP can expect better electron donating than CPDT, but nitrogen in DTP enhanced the donating effect. Fluorinated TT was made from a polymer with a narrow bandgap and a conjugated polymer with a stable quinoid structure. By narrowing the bandgap with TT, the bond length alternation in the conjugation ring system can be controlled, resulting in a low bandgap polymer. Through this, the absorbance of PDTPTT and PCPDTTT was observed at 500-900 nm. Absorbances of 667 and 660 were obtained in the solution state, and 678 and 696 nm were obtained in the film state. PCPDTTT became more red shift than PDTPTT. In addition, the optical bandgap of 1.27eV and 132eV, PDTPTT showed a low bandgap, which shows stronger electron-donating properties of PDTPTT. The energy bandgap was -3.5eV and -3.5eV for HOMO, -4.7eV and -5.1eV for LUMO, respectively, showing bandgap of 1.2eV and 1.6eV. however PCPDTTT showed deep HOMO energy level and 1.6eV band gap, A close to 1 linear relationship between Pin and Jph indicates the minimized bimolecular recombination process that promotes charge transfer and fast signal response in OPDs. Phtodetecting properties yielded decectivity of 1.52 X 10^11 jones and 1.14 X 10^12, and PDTPTT showed poor on/off ratio due to high dark current density.

Poster Presentation : **POLY.P-72**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Synthesis Method of Ladder-like Polysilsesquioxane of Trifluoropropyltrimethoxysilane with Controllable Molecular Weight

Jong-tak Lee, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

Polysilsesquioxanes(pssq) have cage, ladder and random structures. In this study, trifluoropropyltrimethoxysilane was used to synthesize ladder-like pssq to study molecular weight control according to the polymerization time. Pssq synthesis was carried out at room temperature, and stirring time was set from 36 hours to 120 hours. After synthesis, a solution in the form of a resin was obtained through layer separation. The synthesized pssqs were characterized by Si-NMR, GPC, and XRD. As a result of GPC analysis of the synthesized pssqs, the molecular weight could be adjusted from 780 to 5117 based on the mass average molecular weight. The synthesized pssqs were coated on glass to measure the water contact angle, and it was confirmed that the higher the molecular weight, the higher the water contact angle.

Poster Presentation : **POLY.P-73**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Thermal Response of Laponite-containing Poly(N-isopropylacrylamide) Nanocomposite Hydrogels

Daewon Sohn[*], Younhee Jeong

Department of Chemistry, Hanyang University, Korea

Typical N-isopropylacrylamide (NIPAM)-based hydrogels have various applications because of their thermo-sensitivity around Lower critical solution temperature (LCST). In this study, Laponite-poly(N-isopropylacrylamide) (PNIPAM) gels were synthesized with different concentrations of clay. The temperature dependence of NIPAM showed a dramatic change in the adsorbability of water. NIPAM monomers tend to expand below the LCST and shrink above the LCST. The hydrogels composed of laponite contributed to improved mechanical properties, confirmed by swelling tests, compare with the hydrogels of PNIPAM only. The gels were evaluated by using differential scanning calorimetry (DSC) measurements in the dried state. The remarkable change took place at 35°C in all DSC thermograms. A dynamic light scattering (DLS) experiment was also performed to investigate the crosslinked interactions of PNIPAM and laponite. Consequently, the main factor of enthalpy change was related to a clay-polymer network structure affected by the changes in temperature.

Poster Presentation : **POLY.P-74**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Additive-Controlled Lyotropic Liquid Crystalline Phase Behavior of Amphiphilic Random Copolymer Solutions

Shaheen Pathan, Minjoong Shin[1], Myungeun Seo[2,*]

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

Lyotropic liquid crystals have grabbed attention. Typically, amphiphilic molecules contained hydrophilic and hydrophobic (head/tail) groups, self-assembled in water to form a variety of nanostructures. Compared to this noncovalent "supramolecular polymerization" pathway, copolymerization of hydrophobic and hydrophilic monomers offers new opportunities to control the phase behavior by adjusting the sequence of repeating units. As the self-assembling length scale is primarily correlated to the pendant group size, this approach is also distinct from block copolymers showing the backbone length-dependent scaling. Here, we introduce additives as another parameter to further tune the lyotropic phase behavior of amphiphilic random copolymer solutions. How the additive-pendant interaction will affect the phase behavior will be discussed compared to the pristine polymer solution.

Poster Presentation : **POLY.P-75**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Synthesis of A-A Type Conjugated Polymers with a Strong Electron-Accepting Distannylated Monomer

Sang Young Jeong, Han Young Woo[1,*]

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

Many research groups have reported synthesized n-type conjugated polymers using the acceptor-acceptor (A-A) strategy to realize n-type performance. A-A type copolymerization is an effective strategy to develop high-performance n-type conjugated polymers which directly connects the electron-deficient building blocks to decrease HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) energy levels. Also the absence of ICT (intramolecular charge transfer) characteristics in A-A type conjugated polymers would facilitate the more delocalized charge carrier species. However, the disadvantages are more critical. First, the resulting polymers always show low molecular weights and high degree of structural defects. Although synthesized through many coupling reactions, electron-deficient building blocks are less reactive. Second, distannylated monomers of electron-accepting building blocks are usually unstable and are difficult to synthesize, because distannylated monomers are difficult to purify. Therefore, it is important but challenging to design distannylated monomers of electron-accepting building blocks and prepare A-A type polymers with high molecular weight.Recently, a distannylated electron-deficient bithiophene imide (BTI-Tin) monomer was synthesized and reported by Guo group.BTI-Tin has a very high reactivity in the stille coupling reaction and the resulting A-A type polymer has a high molecular weight. In this work, we synthesize BTI-TiN as a distannylated monomoer and applied it into the synthesis of A-A type polymers with stille coupling. We adopted IDT derivates as the dibromo monomer. IDT derivates possesses strong and broad absorption, low LUMO and HOMO energy levels, good electron transport ability. Therefore, we synthesized new A-A type polymers by combining BTI-Tin and IDT derivates through a stille coupling reaction.In further research, we will study the relationship between molecular structure, physical properties and identify device characteristics by fabricating organic solar cell device.

Poster Presentation : **POLY.P-76**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Develop of indacenodithiophene based non-fullerene acceptors for OPV

Yeong Heon Jeong, Yun Hi Kim[1,*]

Department of chemistry, Gyeongsang National University, Korea

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

Non-fullerene acceptors (NFAs) for OPV based on indacenodithiophene (IDT) were synthesized and their material properties and OPV device properties were measured. H-aggregation was prevented by using the side chain of the meta-site alkoxyalkylphenyl group, and the maximum absorption wavelength was redshifted compared to 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno [2,3-d:2′,3′-d′]-s-indaceno[1,2-b:5,6-b′]dithiophene (ITIC)-acceptor by introducing a π-bridge. In addition, OPV blended with donor polymer showed sufficient performance by synthesized NFAs.

Poster Presentation : **POLY.P-77**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

The enhanced gas adsorption capacity of hybrid composites of selectively modified clay nanotubes and metal-organic frameworks

HyeYeon Cho, Daewon Sohn*

Department of Chemistry, Hanyang University, Korea

In this study, the surface of halloysite nanotubes was modified selectively and hybrid materials were synthesized with the modified nanotubes and metal-organic frameworks (MOFs). Halloysite has different electric charges inside and outside the tube, so it can be selectively modified as needed, thereby inducing differentiated characteristics. Herein, modified HNTs were used for gas adsorption with MOFs, HKUST-1, the most widely studied MOFs owing to their high porosity. MOFs were loaded into the lumen of the acid-modified HNTs, EHNT, and HNT-NH_2. After all synthesis via the solvothermal method, the final product was named EHNT@HKUST-1, HNT-NH_2@HKUST-1.The gas adsorption capacity was analyzed by Brunauer-Emmett-Teller (BET) using N_2 and CO_2 gases. Specifically, the EHNT@HKUST-1 composite showed enhanced CO_2 gas adsorption capacity compared to HNT@HKSUT-1, being increased about 14.9 times, from 8.344 cm^3(STP)g-1 to 19.332 cm^3(STP)g-1. Additionally, HNT-NH_2@HKUST-1 indicated around 24.849 cm^3(STP)g-1 of CO_2 gas adsorption capacity. The morphological and structural characteristics were also analyzed by SEM, TEM-EDS, and XRD. By the confined tube structure of HNTs, MOFs could be synthesized along the HNTs longitudinal axis.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **POLY.P-78**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Investigation of Thiophene Spacer at Benzodithiophenedione(BDD) Based Polymer Donors for Non-Fullerene Organic Solar Cells (OSCs)

Suha Lee, Do-Hoon Hwang[1,*]

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

In this study, polymer donors used in active layer based on benzo[1,2-*c*:4,5-*c*']dithiophene-4,8-dione (BDD) were synthesized, which showed good efficiency as an accepting unit in the D-A type donor. We designed and synthesized PBDT-biBDD based on BDD unit and used it as a polymer donor. However, it shows moderate efficiency. The reason for this is that the intermolecular distortion has increased due to the interaction between BDD was introduced between BDD molecules. UV-vis absorption region was red-shifted as a change in the energy bandgap, resulting in complementary absorption with the non-fullerene acceptor material. The device of inverted structure (ITO/Zno/Polymer:IT-4F/MoO_3/Ag) was produced to measure photoelectric properties. As a result, PBDT-biBDD_T showed power conversion efficiency (PCE) of 5.99% and PClBDT-biBDD_T showed PCE of 2.50%. Thus, this study has demonstrated that improving intermolecular correctness greatly helps to improve photoelectric properties.

Poster Presentation : **POLY.P-79**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Achieving Blue-wavelength Selectivity with Porphyrin-based OPD Materials

Jaehee Park, In Hwan Jung*

Department of Organic and Nano Engineering, Hanyang University, Korea

We synthesized a polymer OPD material capable of a blue-selective spectrum by suppressing the Q-band absorption of porphyrins. Previous porphyrin-based PD materials have rarely been used as OPD materials due to their strong Soret and Q-band absorption. We synthesized a porphyrin-based OPD material combining PZn with an FL moiety with an alkyl chain. The FL moiety suppressed the absorption of the Q-band, showing excellent blue wavelength selectivity in OPD. The alkyl chain linked to the FL moiety was perpendicular to the planar backbone structure of PZn-FL, which prevents aggregation between PZn molecules and is suitable for achieving a narrow peak with FWHM of 45 nm in the film state. In addition, the planar backbone structure of PZn-FL achieved excellent hole and electron mobility of 4.2 x 103 and 2.0 x 10.4 cm2/Vs,and these excellent hole transport properties are attributed to the electron donating properties of PZn-FL.

Poster Presentation : **POLY.P-80**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Formulation of photo-responsive 3D printable inks: gold nanorods-hydrogel nanocomposites for soft actuator fabrication

Monica cahyaning Ratri, Jungju Ryu[1], Kwanwoo Shin[2,*]

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

Various types of Nanocomposite hydrogel ink formulation for innovative material purposes is a strategy in the biomedical, pharmaceutical, soft robotic, and tissue engineering fields. With the combination of stimuli-responsive nanocomposites and 3D printable matrix properties, bio-inspired soft actuators have been fabricated in the presence of various external stimuli. The recent stimuli-responsive soft actuators need a long time to generate the actuation process, and the actuation process is mainly conducted inside the water. To overcome the current limitation, we formulated and tested PNIPAAm-gold nanorod composites as an ink material to fabricate the heat-sensitive soft actuators for photo-responsive soft robotic motions. By adding PEG-SH coated gold nanorods in the active ink, this metallic nanorod can absorb the near-infrared (NIR) light and release heat to its surroundings due to its surface plasmon resonance (SPR). Active ink made from Poly (N-isopropyl acrylamide) (PNIPAAm) will generate a self-morphing process based on its temperature-sensitive properties if there is heat in its surroundings. The waterless system is one of the advantages because the noncontact external stimuli can induce local heat generation faster. By controlling the addition of PEG-SH coated gold nanorods in the active ink and the intensity of NIR light, we can control the heating and actuation process of the system. We will present our preliminary results to formulate the nanocomposite ink and photo-responsive reactions of the 3D printed soft actuators.

Poster Presentation : **POLY.P-81**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Tunable Wetting of Superomniphobic Surface Structures Based on Shape Memory Polymers

Anwoo Jeong, Seung Goo Lee*

Department of Chemistry, University of Ulsan, Korea

Shape memory polymer (SMP) shows reversible shape change through external stimuli such as heat, light, electricity, and magnetism. SMP is widely used in various fields including medical circles, sensors, and electronics. The superomniphobic surfaces display high liquid contact angles as well as low liquid contact angle hysteresis, which result from low surface energy and re-entrant surface structures. Such surfaces have a range of commercial applications, including self-cleaning, non-fouling, stain-free clothing, drag reduction, corrosion prevention and separation of liquids. In this work, we investigated the tunable wetting behavior of superomniphobic surface structures using a thermo-responsive SMP. Superomniphobic surface structures were prepared by replica molding of SMPs based on bisphenol A diglycidyl ether. We measured contact angle and contact angle hysteresis, and as a result, we found that the Cassie state was maintained for water(θ = 163°, θ_{CAH} = 38°) and hexadecane(θ = 154°, θ_{CAH} = 46°). Heat and pressure were used to change the shape and then reheat it again to restore the shape. It was confirmed that existing water/oil-repellent surface properties were maintained after shape restoration. These structures are expected to be available in various fields such as biosensors and liquid transport systems.

Poster Presentation : **POLY.P-82**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Characterization of catechol modified PEG gels controlled by crosslinking units

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*

This study explores the influences of crosslinking geometry on the structure of gel networks. The various crosslinking units were employed by catechol mediated reactions. The end groups of PEG chains were modified with catechol moieties, and then the crosslinking was established by pH controls which can provide various crosslinking geometries: linear links and triangular linkages. The gels were characterized with UV spectroscopy, light scattering, and small-angle X-ray scattering measurements. The crosslinking geometries were probed by UV measurements. The polymer concentration effects were determined through the dynamic behaviors of polymer chains in solutions. X-ray scattering reveals the nano structures of polymer networks depending on crosslinking geometries. We found two important factors related to the gel's characteristics: polymer concentrations and oxidant moieties (i.e., iron cations). The results provide the insights that can develop novel hydrogels with facile synthetic routes.

Poster Presentation : **POLY.P-83**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Alkyl-Side-Chain Engineering of Nonfused Nonfullerene Acceptors with Simultaneously Improved Material Solubility and Device Performance for Polymer Solar Cells

Guseon Kim, Eunhee Lim[1,*]

University of Seoul, Korea
[1]Department of Applied Chemistry, University of Seoul, Korea

Two nonfullerene small molecules, TBTT-BORH and TBTT-ORH, which have the same thiophene−benzothiadiazole−thiophene (TBTT) core flanked with butyloctyl (BO)- and octyl (O)-substituted rhodanines (RHs) at both ends, respectively, are developed as electron acceptors for polymer solar cells (PSCs). The difference between the alkyl groups introduced into TBTT-BORH and TBTT-ORH strongly influence the intermolecular aggregation in the film state. Differential scanning calorimetry and UV−vis absorption studies reveal that TBTT-ORH exhibited stronger molecular aggregation behavior than TBTT-BORH. On the contrary, the material solubility is greatly improved by the introduction of a BO group in TBTT-BORH, and the inevitably low molecular interaction and packing ability of the as-cast TBTTBORH film can be effectively increased by a solvent-vapor annealing (SVA) treatment. PSCs based on the two acceptors and PTB7-Th as a polymer donor are fabricated owing to their complementary absorption and sufficient energy-level offsets. The best power conversion efficiency of 8.33% is obtained with the SVA-treated TBTT-BORH device, where, together with a high open-circuit voltage of 1.02 V, the charge-carrier mobility and the short-circuit current density were greatly improved by the SVA treatment to levels comparable to those of the TBTT-ORH device because of the suppressed charge recombination and improved film morphology. In this work, the simultaneous improvement of both material solubility and device performance is achieved through alkyl side-chain engineering to balance the trade-offs among material solubility/crystallinity/device performance.

Poster Presentation : **POLY.P-84**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Chemodegradable liquid crystalline epoxy thermoset based on azomethine mesogen core

En Trinh Thi, Hyeonuk Yeo[1,*]

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

Conventional epoxy resins have random network structure, so its thermal properties like heat insulators. To improve the thermal conductivity of liquid crystal epoxy resins (LCEs), we change the random structure by highly oriented one. It leads to the material can dissipate heat faster by reducing phonon scattering phenomenon. Many researches indicate that LCEs with mesogens contain azomethine group when curing with suitable curing agents can form highly alignment structure network. As a result, its thermal conductivity increases dramatically.In this research, various mesogens bearing azomethine group with different numbers of carbon in the extender were synthesized then cured with the aromatic diamine curing agent. The structure of mesogens, the chemical and optical properties as well as the thermal properties of fabricated products were determined by different analysis methods like NMR, MS, TGA, POM, XRD and thermal conductivity. All of the monomers show typical nematic phases and thermal conductivity of cured ones increase when the number of carbon in spacer go up but the glass transition temperatures (Tg) reduce when the carbon chains were extended. The details their chemical decomposition properties will be discussed in the presentation

Poster Presentation : **POLY.P-85**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Hydrogen Bonding Effect on AIE-activity of Acylhydrazone-based Conjugated Microporous Polymers, and Their Application to Nitroaromatic Compounds Detection

Inhwan Cha, Seohyun Baek, Kyung-su Kim*, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Acylhydrazone-based fluorescent conjugated microporous polymers (CMPs) were presented and their emissive properties were controlled by inter- and intra-hydrogen bonding. The synthesized two types of CMP, which were made from 1,3,5-triformylbenzene with Terephthalic dihydrazide **(BH-CMP)** or 2-Amino-1,4-benzenedicarboxylic acid 1,4-dihydrazide **(ABH-CMP)** were characterized by FT-IR spectroscopy, XRD, solid-state NMR spectroscopy, and photoluminescence spectroscopy. Interestingly, **BH-CMP** exhibited emission enhancement via adsorption of water molecules, while **ABH-CMP**, which possesses free amine groups, showed emission decrease upon the addition of water molecules. We found that the differences in emission trends of **BH-CMP** and **ABH-CMP** for water molecules originate from different hydrogen bonding networks with water molecules in each CMP. We also applied acylhydrazone-CMPs to the detection of nitroaromatic compounds, especially 1,3,5-trinitrotoluene (TNT). We confirmed that **ABH-CMP** suspension in DMF exhibited high selectivity for TNT compared to other nitroaromatic compounds such as nitrobenzene, 4-chloronitrobenzene, 2,3-dichloronitrobenzene, and 2,4-dinitrotoluene.

Poster Presentation : **POLY.P-86**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Biocompatible Metal-Sensing Polymers Based on Terpyridine-Functionalized Polysuccinimides

Ju-Young Choi, Hwi Hyun Moon, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

The Detection of metal ions is essential because they are toxic and pollutants in the environment and human body. The presence of metal ions can be sensing by spectroscopic changes. Transition metal ions such as Ni^{2+}, Co^{2+}, Fe^{2+}, and Zn^{2+}, form a metal-ligand complex through coordination with terpyridine. Poly(succinimide) (PSI) is synthesized by aspartic acid, a type of amino acid, also it has bio-friendly and non-toxic properties. PSI can be easily functionalized using aminolysis reaction to form hydrophilic and hydrophobic copolymers. Herein, we have designed and synthesized PSI-Terpyridine (PTP) to detect transition metal ions. PTP is coordinated with metal ions to fluorescence and sense specific metals. The ethanolamine monomer is used as a copolymer with terpyridine to synthesize water-soluble PTP. We expect PTP to be applied to an aqueous phase probe by utilizing its biocompatible properties while detecting metal ions.

Poster Presentation : **POLY.P-87**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Photo-responsive, self-healable, fully bio-based polymers from a dimer acid and a cinnamic acid

Jiyun Kim, Hye Jin Cho, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Currently, the use of renewable resources for sustainable technology is inevitable. Consumers and industry have raised environmental issues, and environmentally friendly alternatives are needed. However, currently used epoxy polymers, especially thermosetting epoxy polymers, cause health and environmental problems. Therefore, this study aims to make a renewable epoxy network polymer using bio-based epoxy monomers. We designed an epoxy network polymer with an epoxy monomer obtained from a dimer acid, which can be easily obtained from vegetable and animal oils and photoreactive plant-derived trans-cinnamic acid. It is expected to be a very eco-friendly route in that it does not use toxic catalysts and solvents. In addition, the C=C bond moiety of the synthesized epoxy polymer is expected to be beneficial for the formation of a self-healable network via photo-induced [2+2] cyclization reaction.

Poster Presentation : **POLY.P-88**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Supramolecular Polymerization with Hydrazone-based Molecular Building Blocks: Solvent-Switchable Chiral Platform

Hye Jin Cho, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Supramolecular chemistry has drawn much attention because it enables a deeper understanding of superstructures observed in nature. Among them, supramolecular polymers with potential in various fields have been reported recently, such as sensing, optical switches, and optoelectronic devices. In particular, it is considered beneficial for circularly polarized luminescence (CPL) by controlling the luminophore arrangement. However, further research on CPL-active materials is required because achieving both high dissymmetry and emission efficiency remains challenging. Herein, we designed benzoyl hydrazone para-pyridinium conjugates which their self-assembled helical nanowires play as a chiral platform for a new CPL system based on hydrazone luminophore. The hydrazone monomers were self-assembled via direct intermolecular interactions, and the chirality of terminal alkyl substituents determined their apparent supramolecular chirality. Interestingly, in water, they were self-assembled around the backbone consisted of structural water molecules via hydrogen bonding. The resultant assembly of hydrazone and water molecules successfully served as a chiral platform for CPL when achiral hydrazone-based luminophore was co-assembled.

Poster Presentation : **POLY.P-89**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Topology effect on thiourea-based hyperbranched polymer electrolytes for lithium-ion battery

Hyejun Kim, Changsik Song*, Kyung-su Kim

Department of Chemistry, Sungkyunkwan University, Korea

Over the past few decades, long-life, high specific-capacity, and environmentally friendly lithium-ion batteries (LIBs) have been widely used in various types of electronic devices and electric vehicles. LIBs typically consist of an anode, cathode, separator, and electrolyte. Most commercially available LIBs use a liquid electrolyte with high ionic conductivity (10−3−10−2 S cm−1), but there are some potential problems including electrolyte leakage and flammability. Gel polymer electrolytes (GPEs) have been considered as promising candidates to replace conventional liquid electrolytes because of their advantages such as thermal and electrochemical stability and good ionic conductivity (~ 10–3 S cm–1). In GPEs, the control of topological structures of polymers is an important and emerging research area in polymer chemistry, can regulate various physical properties of polymers such as molecular weight, solubility, viscosity, and topological cavities. Hyperbranched (HB) polymers, a particular type of polymer architecture, have characteristics with high branching density, compact structure, high solubility, and low intrinsic viscosity. There are two synthetic strategies to prepare HB polymers; the first method is self-condensing polymerization of ABn (n ≥ 2) monomers, the second method is polymerization between A2 and Bn (n ≥ 3) monomers. Among them, the A2 + Bn method has been preferred because the synthesis of A2 and Bn (n ≥ 3) monomers is more accessible than that of ABn (n ≥ 2) monomers. Thiourea can bind anions and form bidirectional hydrogen bonding with various anions and affect activation barriers to ion transport, which motivated us to design thiourea-based GPEs for LIBs. Thiourea molecules have been intensively used as an electrolyte additive in LIBs to form a stable solid electrolyte interface layer on the Li metal electrode, suppressing Li dendrite growth and electrolyte decomposition. However, to the best of our knowledge, the introduction of thiourea-based polymers into GPEs for LIBs has not yet been reported.Herein, we report thiourea-based GPEs with a highly branched topology or intramolecular cyclic topology. We investigated the effect of the branching degree of thiourea-based GPEs on Li-ion conductivity and effect of anion chelation of thiourea on ion-diffusion and -transport.

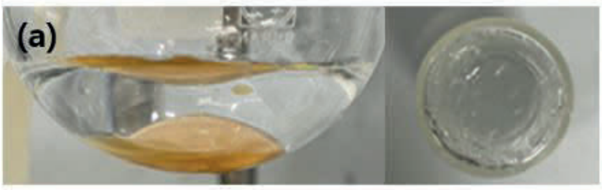
Poster Presentation : **POLY.P-90**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

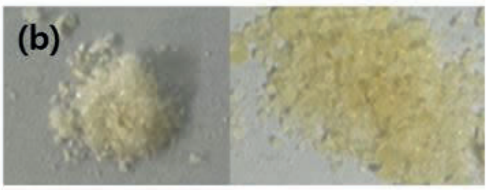
Synthesis and characterization of ionic polymers containing bis-pyrrolidinium pendants

Jung Min Kim, Minjae Lee*

Department of Chemistry, Kunsan National University, Korea

Ionic polymers containing bis-pyrrolidinium cations as a pendant are synthesized and characterized. Polymerizable methacrylate group is introduced to the monomers of C_4-bridged bis-pyrrolidinium salts with different linear alkyl chain tails. Free-surfactant emulsion polymerization method with a water soluble initiator $K_2S_2O_8$ is used to synthesize the ionic polymers. The polymerization reaction completions are confirmed by FT-IR; the vinyl peaks from the monomers at 1650 cm^{-1} disappeared. Polymerization conditions are 1) monomer and initiator ratio 3:1, 2) chloroform and DI water ratio 1:20, and 3) reaction temperature 90 ℃. Different monomer to initiator ratio 10:1 does not work well and a lot of monomers remains. The thermal properties of the synthesized ionic polymers are studied by differential scanning calorimetry and thermal gravimetric analysis. Especially, the bis-pyrrolidinium polymer with n-propyl pendant tail shows crystalline morphologies on polarized optical microscope images at room temperature.





Poster Presentation : **POLY.P-91**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Biomass-derived Furanic Dienes: Diels-Alder Reaction-mediated Supramolecular Gels

Byounghyun Kim, Juhyen Lee, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Polyurethane (PUs) is a major engineering material with excellent heat resistance and rubber-like elasticity, mostly synthesized from petroleum-based resources which lead to environmental pollution. Furfuryl materials can be easily obtained from lignocellulose, which can be applied as a sustainable material such as biomass-derived polymer platforms. This eco-friendly platform can be used to form supramolecular gels or network polymers, and its physical properties can be controlled through the Diels-Alder (DA) reaction. In this study, a carbamate group was introduced directly at the C-2 position in furan. By lowering the energy level due to the electron-donating effect, this structure showed an improved DA reaction rate compared to the structure in which substituted a methylene group. In addition, a supramolecular gel is formed through intermolecular interaction between DA adducts, which has a different gelation rate due to the conformation according to various maleimides. Furthermore, self-healing using the DA reaction can be applied to the eco-friendly film and coating industry.

Poster Presentation : **POLY.P-92**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Development of Biomass-derived Polyurethanes using a Versatile Polymer Platform towards Photodegrability and Non-flammability

Juhyen Lee, Seohyun Baek, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Polyurethanes (PUs) are one of the most interesting polymers, which are generally synthesized from petroleum-based materials. Furandicarboxylic acid (FDCA) obtained from 5-hydroxymethylfurfural (5-HMF) has been considered a good biomass precursor due to good thermal stability and physical properties. In this study, we present a novel furan-based polymer platform, furandiacylazide (FDAz), from FDCA. Using FDAz, we successfully synthesized poly(furanyl-urethane-isocyanurate)s (PFUIs) through a thermal Curtius rearrangement. Also, the nitro group was introduced at the ortho position of PFUI to obtain photo-degradable property. We measured photo-degradability of biomass-derived polyurethane and confirmed potential as an eco-friendly plastic. Tuning the polymerization conditions enabled control of the relative ratios of the urethane and isocyanurate moieties, which presented good heat-resistance of a fully isocyanurate-contaning polymer. FDAz is a versatile polymer platform that can be applied to the synthesis of various eco-friendly potential polymers (PFUIs).

Poster Presentation : **POLY.P-93**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Norbornene-based bottle-brush polymers with enhanced lubricating properties

Changsik Song*, Hwi Hyun Moon

Department of Chemistry, Sungkyunkwan University, Korea

Recently, bottle-brush polymers are widely used for the studies of hydration lubrication due to their unique mechanical and rheological properties. By mimicking lubricin we synthesized bottle-brush polymers using two polymerization methods: ring opening metathesis polymerization (ROMP) and reversible addition fragmentation chain transfer (RAFT) polymerization. To do so, norbornene and chain transfer agent (CTA) containing monomers (Styrne, 2-Hydroxyethyl methacrylate; HEMA) were used for ROMP and RAFT, respectively. Especially, HEMA is widely know as major monomer used in soft contact lenses and has excellent biocompatibility and blood compatibility. The molecular weight of the synthesized polymer was measured by a GPC and calculated percent conversion using NMR. The lubricating properties of the synthesized brush polymers affected by bottle-brush architecture and hydrate state were examined by a ball on disk. The friction coefficient is different measured in water and dry condition by polymers properties.

Poster Presentation : **POLY.P-94**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Biomass-Derived, Carbon Dioxide-Immobilized Polyurethane Networks with Self-Healable and Reprocessable Properties

Seohyun Baek, Juhyen Lee[1], Inhwan Cha[1], Changsik Song[1,*]

Polymer Synthesis Lab., Sungkyunkwan University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Today, global warming and various environmental problems are getting serious because of the greenhouse effect caused by increased carbon dioxide. Recently, the studies of biomass-derived materials such as HMF, BHMF, ISB, and FDCA, etc., and CO2 utilization have been conducted as a solution to the environmental problems. Among them, recyclable eco-friendly polyurethane or other polymer has a wide range of applications and needs research. Biomass-based networks which have thermal stability and recyclability is suitable for application of eco-friendly polymers. In this study, we synthesized a biomass-derived polyurethane networks (PU networks) using a novel furan carbonate diol (FCD-R) in eco-friendly methods. The synthesis of FCD-R was performed by introducing carbon dioxide directly into BHMF. Using mechanochemical synthesis (Ball-milling), the PU networks was made from FCD-R, erythritol, and diisocyanate. The film was fabricated using hot press and performed self-healing properties by exchanging dynamic covalent bonds. The thermal properties of the networks were measured by TGA, DSC, DMA, UTM and rheometer. Accordingly, PU networks, a polymer network that can be recycled by heating even if it is damaged, is expected to be effectively used in various fields and will contribute to solving environmental pollution problems.

Poster Presentation : **POLY.P-95**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Flexible and Semi-Transparent Top-Contact Structure Organic Electrochemical Transistors based on Ultra-Thin Au/PEDOT:PSS Hybrid Electrode for Human Skin Electronics

Il-Young Jo, Myung-Han Yoon*

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

Organic electrochemical transistors (OECTs) are one of the most promising device platforms for the field of bio-healthcare electronics because it have several advantages including high transconductance, low voltage operation, and long-term stability. Here, we suggest an ultra-thin hybrid electrode was fabricated by thermally depositing ultra-thin Au electrode on crystalline poly(3,4 ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) thin film, which has a transmittance of up to 55 % at visible range wavelength and low sheet resistance of 23.12 Ω/sq. Based on this structure, a semi-transparent and flexible top-contact structure OECT was fabricated that shows a transconductance of 1.6 mS, and the performance was maintained even in the highly bending state. Finally, this semi-transparent OECT is attached to human skin to successfully perform ECG measurements.

Poster Presentation : **POLY.P-96**

Polymer Chemistry

Exhibition Hall 1 THU 11:00~12:30

Fabrication of compression bandage with trimethoprim-loaded polyvinyl alcohol nanofibers for preventing secondary infection

Sangwoo Lee, Myung-Han Yoon*

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

Compression bandages are one of the effective first aid and treatment tools for traumatic injuries such as abrasions, bruises, laceration, and fractures. However, in actual use, as time goes by, because of inadequate maintenance of hydration staten clotting of wounded area or secondary infection can be happened with growth of harmful bacteria. We introduce drug-loaded polyvinyl alcohol (PVA) nanofibers which can maintain water retention and inhibit growth of bacteria on compression bandages. After crosslinking using citric acid (CA) on a PVA-based hydrogel, and loading an antibiotic called Trimethoprim (TMP), it will be coated on a cellulose-based compression bandage through electrospinning. Due to the mechanism by which TMP is released, bacterial inhibition on the skin occurred. In addition, by controlling the amount of thermal crosslinking time and drug loading, the drug releasing rate could also be controlled

Poster Presentation : **POLY.P-97**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Tris(4-(1-phenyl-1H-benzo[d]imidazole)phenyl)phosphine oxide for Enhanced Mobility and Restricted Traps in Photovoltaic Interlayers

Doyeong Choi, Yun Hi Kim[1,*]

Department of Materials Engineering and Convergence Technology, Gyeongsang National University, Korea

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

As small molecule organic materials, Tris(4-(1-phenyl-1H-benzo[d]imidazole)phenyl)phosphine oxide (TIPO) and Tris(4-(1-phenyl-1H-benzo[d]imidazole)phenyl)triazine (TBIT) were newly synthesized and applied to n-type interlayer of planar perovskite solar cells (PSCs) for effective electron transport layer. The molecule materials contained phenyl benzimidazole group which is combined with a phosphine oxide core or triazine ring core and has contributed to the enhancement of charge extraction and stability. Since the constituent molecules phosphine oxide and benzimidazole (BIZ) have high polarity and strong π-electrons, the molecules trigger passivation defects to improve charge transport and flattening the surface morphology. In addition, the stability of the device was improved by introducing TIPO material as the passivation and protection layer. This electron extraction analysis, electrical resistance analysis and surface morphology investigation were verified by space charge limited current (SCLC), photoluminescence (PL), impedance, and atomic force microscopy (AFM) analysis.

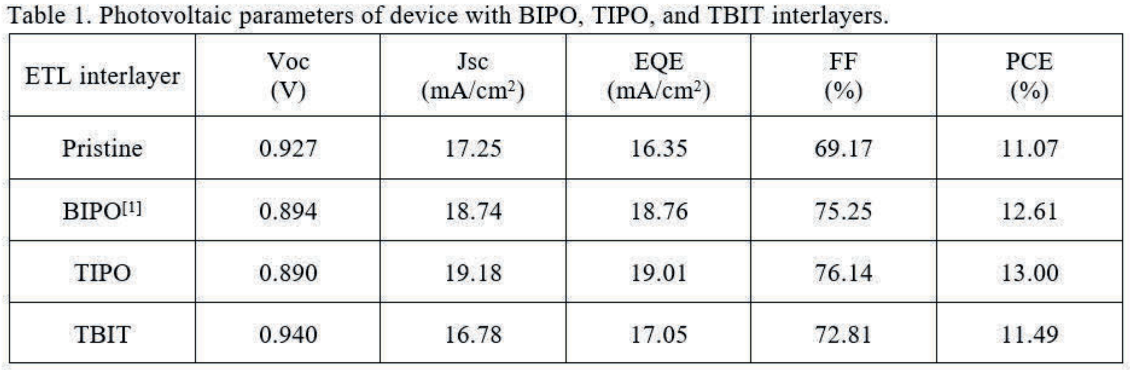


Table 1. Photovoltaic parameters of device with BIPO, TIPO, and TBIT interlayers.

ETL interlayer	Voc (V)	Jsc (mA/cm^2)	EQE (mA/cm^2)	FF (%)	PCE (%)
Pristine	0.927	17.25	16.35	69.17	11.07
BIPO[1]	0.894	18.74	18.76	75.25	12.61
TIPO	0.890	19.18	19.01	76.14	13.00
TBIT	0.940	16.78	17.05	72.81	11.49

Poster Presentation : **POLY.P-98**
Polymer Chemistry
Exhibition Hall 1 THU 11:00~12:30

Efficient, Thermally Stable, and Mechanically Robust AllPolymer Solar Cells Consisting of the Same Benzodithiophene Unit-Based Polymer Acceptor and Donor with High Molecular Compatibility

Cheng Sun, **Yun Hi Kim**[1,*], **Soon-Ki Kwon**[2,*], **Taek-Soo Kim**[3,*], **Bumjoon Kim**[4,*]

Department of chemistry, Gyeongsang National University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*
[2]*Gyeongsang National University, Korea*
[3]*Korea Atomic Energy Research Institute, Korea*
[4]*Department of Chemical Engineering & Biotechnology, Korea Advanced Institute of Science and Technology, Korea*

All polymer solar cells (all-PSCs) are a particularly attractive class of photovoltaics for the wearable and portable applications due to their excellent morphological and mechanical stabilities. To enhance their power conversion efficiency (PCE), new types of polymeric acceptors consisting of non-fullerene small molecule acceptors (NFSMA) capable of large light absorption with high charge carrier mobility has been recently proposed. However, polymerization of the NFSMA greatly reduces the entropy of the mixing in the PSC blends, which prevents the formation of properly-intermixed blend domains that is required for efficient charge generation and mechanical robustness. Herein, we provide an important guideline to design efficient polymeric acceptors (PA) having the same building unit with polymer donor (PD), which significantly enhance the morphological compatibility of all-PSCs. We prepare a series of new NFSMA-based PA [P(BDT2BOY5-X), (X = H, F, Cl)] that contain the benzodithiophene (BDT) unit. Thus, all-PSC blends composed of PBDB-T PD and P(BDT2BOY5-X) PA, both of which contain BDT units, exhibit excellent interfaical compatibility and morphological properties. As a result, the PBDB-T:P(BDT2BOY5-Cl) all-PSCs show significantly enhanced PCE of 10.84% compared to Y5-2BO NFSMA (PCE = 7.02%) and conventional PA P(NDI2OD-T2) (PCE = 6.00%). More importantly, the improved compatibility between PD and PA greatly enhances the mechanical robustness of all-PSCs. Crack onset strain (COS) and toughness of the PBDB-T:P(BDT2BOY5-Cl) blend are 15.9% and 0.32 MJ m-3. Our new design of

NFSMA- and BDT-based PA materials provides excellent morphological compatibility between PA and PD, leading to high mechanical robustness and PCE of all-PSCs.

Poster Presentation : **IND.P-1**
Industrial Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Structure Effect of Thermal Initiator to Curing Behavior of Epoxy Resin via Cationic Polymerization

Kim Seungjun

Department of Chemistry and Chemical Engineering, Inha University, Korea

Cationic polymerization is widely employed for the polymerization of epoxy compounds which is typically utilized for adhesives. For example, an anisotropic conductive film (ACF) is an organic film consisting of an epoxy resin, a curing agent, and a conductive particle. ACF is a material inserted between the circuits to be heated and pressurized to adhere both circuits. Temperature for initiation is critical as too much heat negatively affects the performance of the circuit. Lowering the initiation temperature is not always suitable due to instability of the initiator that leads to undesirable curing of the epoxy resin before actual use. Therefore, thermal cationic initiators effective only under desirable conditions are essential for target applications. Herein, we investigated how structural variation in thermal-latent curing agent based on a cationic polymerization mechanism affects initiation and curing behaviors. The initiators with the systematically varied molecular structures were successfully synthesized. The differences in curing behaviors of the thermal cationic initiators for a certain epoxy resin, and their stability were thoroughly studied using differential scanning calorimeter and viscosity measurements.

Poster Presentation : **IND.P-2**
Industrial Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Elucidation of Structure-Property Relationships in Phenylimidazolinato Ir(III) Complexes for Phosphorescence Color-Tuning

Sanghun Lee, Min Su Choe, Yunjeong Seo, Sang Ook Kang, Ho-Jin Son[*]

Department of Advanced Materials Chemistry, Korea University, Korea

The photophysical and electrochemical properties of a series of iridium(III) complexes (**TPIF**, **ITPIF**, **TPICN**, and **ITPICN**) containing a terphenyl or isoterphenyl-substituted phenylimidazole ligand, which bear electron-withdrawing fluoro (–F) or cyano (–CN) groups onto the para-site of the C-phenyl ring, have been synthesized and investigated. F-substituted complexes (**TPIF** and **ITPIF**) exhibited strong absorption band and emissive energy than that of the cyano-substituted complexes (**TPICN** and **ITPICN**). Steady-state photophysical analysis and computational studies reveals that the complexes possess both metal-to-ligand charge-transfer (MLCT) localized on the metal and phenylimidazole and intraligand charge-transfer (ILCT) states originating from the charge transfer from the terphenyl moiety to the phenylimidazole portion. Interestingly, the ordering of the ILCT and MLCT trantision state have been controlled by modulating the electron-withdrawing substituents (–F or –CN), resulting in significantly red-shifted emission at 298K as well as solvent polarity-dependent properties in CN compounds with strong CT characters. All of the terphenyl modified 2-phenylimidazole iridium complexes showed their quantum yields within the range of 33~50%. And the terphenyl group helped iridium metal center avoid proceeding non-radiative process. It was revealed that the EWG of the cyclometalated phenylimidazole ligands contributes substantially to both the HOMO and LUMO of the iridium complexes, the concurrent introduction of an –F and –CN groups on the phenyl ring relative to the Ir metal may lead to a favorable synergetic substituent effect on the color-tuning direction. This may represent a facile yet effective molecular design strategy for Ir(III) complexes with a desirous emission color.

Poster Presentation : **IND.P-3**
Industrial Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Functionalization of Phosphorescent Ir Complexes by Incorporating Terphenyl Periphery Group for Blue PHOLED

Sanghun Lee, Yunjeong Seo, Daehan Lee, Sang Ook Kang, Ho-Jin Son[*]

Department of Advanced Materials Chemistry, Korea University, Korea

We report a series of cyclometalated iridium(III) complexes, Ir(C^N)$_3$, substituted for terphenyl moiety with a sterically shielded strategy based on phenyl-imidazole, which exhibits wide band-gap properties for application to deep-blue phosphorescent OLED devices. The Ir(C^N)$_3$ complexes involve attaching a methyl, phenyl, terphenyl, and isopropyl-terphenyl group to the parent phenylimidazole ligand, abbreviated as **MI**, **PI**, **TPI**, and **ITPI**, respectively. Additional iridium complexes, **TPIF** and **ITPIF**, are also prepared in which the phenyl moiety of phenylimidazole was modified with electron-withdrawing substituents (e.g., -F). It is turned out that a terphenyl molecular fragment not only elevated LUMO but also increased emission quantum yield significantly. All of the terphenyl modified 2-phenylimidazole Ir(III) complexes showed their quantum yields within the range of 33 to 50% and their values were at least three times higher than that found in **MI** complex ($\Phi_{em} = 10\%$), which means that the terphenyl group can effectively prevent the non-radiative process of the iridium(III) complex. With terphenyl modification and further color tuning by adding fluorine and isopropyl groups, **ITPIF** showed blue phosphorescence at 456 nm as well as high quantum yields (40% in solution and 76% in PMMA film). This **ITPIF** complex is selected as a dopant material in the structure of blue phosphorescent organic light-emitting diodes. The highly efficient blue OLED can be realized with a maximum EQE of over 16.4% with CIE value of (0.18, 0.27). Our results demonstrate that bulky substituents are excellent candidates for the achievement of efficient phosphorescent materials and corresponding OLED devices.

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

Industrial Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Electrospun chitosan-stabilized Prussian blue nanoparticles/poly(vinyl alcohol) nanofibers for reactive oxygen species scavenging and wound healing

Dongwan Son, HoIk Lee[1,*], Myungwoong Kim[*]

Department of Chemistry, Inha University, Korea
[1]*Korea Institute of Industrial Technology, Korea*

Nanofiber (NF) mats manufactured in a three-dimensional nonwoven fabric exhibiting very small pores in the scale of tens of nm to hundreds of nm have been utilized for sensors, clothing materials, and dressing materials for wound therapy. However, the single functionality of the NFs fabricated solely from a specific polymer cannot satisfy a variety of desirable applications and needs of consumers, requiring the further development of fiber materials with various functionalities such as antioxidant, antibacterial, and tissue regeneration capabilities. Poly(vinyl alcohol) (PVA) has excellent biocompatibility and mechanical properties and is utilizable as a medical NF material. Chitosan-coated Prussian blue nanoparticles (PB/Chi NP) are effective materials exhibiting outstanding structural stability and in vivo safety, promoting reactive oxygen species (ROS) removal and tissue regeneration. In this study, we demonstrate PB/Chi NP-coated PVA nanofibers (PB/Chi NP-coated PVA nanofiber; PBChi/PVA NF) to improve the antioxidant and tissue regeneration capabilities of PVA NFs. PB/Chi NP-coated PVA nanofibers (PBChi/PVA NF) were successfully fabricated via electrospinning with thorough parameter optimization process. We further show that the resulting hybrid NF system was proven to have excellent biocompatibility, removal of ROS and tissue regeneration capabilities. These NFs will open a valuable route to easily access to anti-aging products, functional cosmetics, medical platform such as wound dressing and prosthetics.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **IND.P-5**
Industrial Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Surface modification of nanocellulose through acetylation reaction

Jeong Seob Byeon, Jaehee Song[1], Yeong-Joon Kim[*]

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

Cellulose, a natural linear polymer, is not soluble in water because of its large molecular weight. Nanocellulose obtained from a strong acid hydrolysis of cellulose can be dissolved in some polar solvents. Nanocellulose has a hydrophilic property due to the presence of hydroxy groups at the glucose units. In this research, in order to reduce the hydrophilicity, the hydroxy groups of the nanocellulose surface were changed to esters through the acetylation reaction. After the reaction, the product was precipitated in polar solvents such as NMP and pyridine, and the acetylation reaction was monitored by Fourier transform infrared spectroscopy.

Poster Presentation : **INOR.P-6**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

[Withdrawal] A novel colorimetric sensor containing anthraquinone derivative for detecting ClO^- and its paper application

Boeon Suh, Jae Sung Heo, Cheal Kim[*]

Fine Chemistry, Seoul National University of Science & Technology, Korea

Poster Presentation : **INOR.P-7**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A functional model for quercetin 2,4-dioxygenase: Geometric and electronic structures and reactivity of a nickel(II) flavonolate complex

Seungwon Sun, Donghyun Jeong[1], Dohyun Moon[2,*], Jaeheung Cho[3,*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*
[2]*Beam Operation Team, Pohang Accelerator Laboratory, Korea*
[3]*Department of Chemistry, UNIST, Korea*

Quercetin 2,4-dioyxgenase (QueD) has been known to catalyze the oxygenative degradation of flavonoids and quercetin. Recent crystallographic study revealed a nickel ion occupies the active site as a co-factor to support O_2 activation and catalysis. Herein, we report a nickel(II) flavonolate complex bearing a tridentate macrocyclic ligand, $[Ni^{II}(Me_3\text{-TACN})(Fl)(NO_3)](H_2O)$ (1) as a functional model for QueD. The flavonolatonickel(II) complex was characterized by using spectrometric analysis including UV-vis spectroscopy, electrospray ionization mass spectrometer (ESI-MS), infrared spectroscopy (FT-IR) and 1H nuclear magnetic resonance spectroscopy (NMR). The single crystal X-ray structure of 1 shows two isomers with respect to the direction of a flavonolate ligand. Two isomers commonly are in the octahedral geometry with a bidentate of flavonolate and a monodentate of nitrate as well as a tridentate binding of Me_3-TACN ligand. The spin state of 1 is determined to be a triplet state based on the Evans' method. Interestingly, electronic configuration of 1 from density functional theory (DFT) calculations revealed that the two singly occupied molecular orbitals (SOMOs) lies energetically lower than the highest (doubly) occupied molecular orbital (HOMO), that is so-called the SOMO-HOMO level inversion (SHI). The HOMO is localized in the flavonolate ligand, and such finding would rationalize that the flavonolate ligand is oxidized first rather than the nickel center. Thermal degradation of 1 resulted in the formation of benzoic acid and salicylic acid, which is attributed to the oxygenation of flavonolate of 1.

Poster Presentation : **INOR.P-8**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Hydride-Transfer Reaction to a Mononuclear Manganese(III) Iodosylarene Complex

Donghyun Jeong, Jaeheung Cho[1,*]

Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Chemistry, UNIST, Korea*

Metal iodosylarene species have received interest because of their potential oxidative power as a catalyst. We present the first example of hydride-transfer reactions to a mononuclear manganese(III) iodosylbenzene complex, $[\mathrm{Mn^{III}(TBDAP)(OIPh)(OH)}]^{2+}$ (**1** ; TBDAP = *N,N*-di-*tert*-butyl-2,11-diaza[3.3](2,6)pyridinophane), with dihydronicotinamide adenine dinucleotide (NADH) analogues. Kinetic studies show that hydride-transfer from the NADH analogues to **1** occurs via a proton-coupled electron transfer, followed by a rapid electron transfer.

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

Inorganic Chemistry

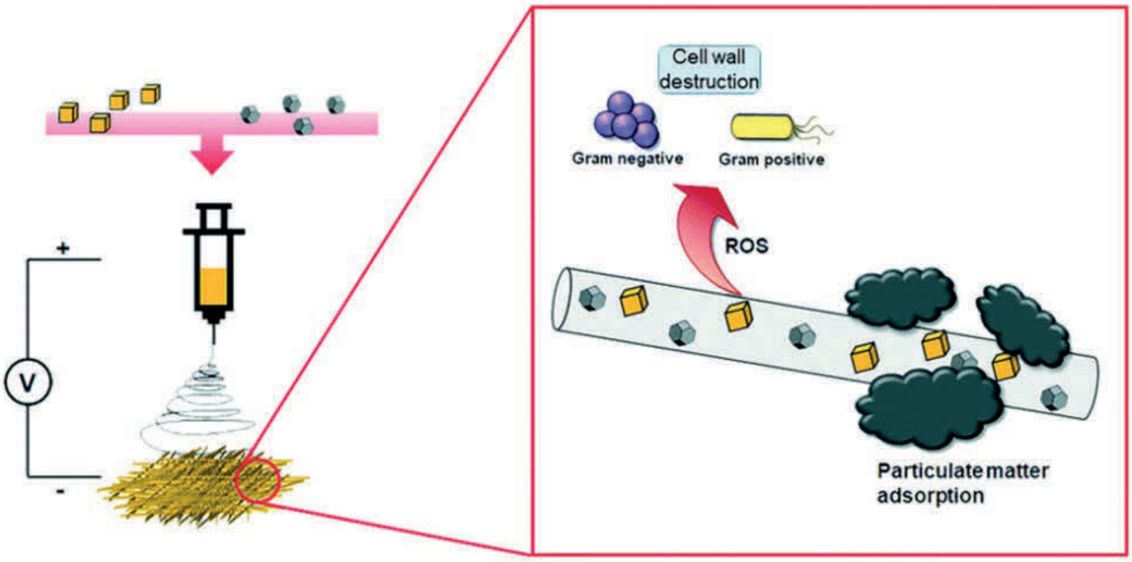
Exhibition Hall 1 FRI 11:00~12:30

Preparation and characterization of multifunctional nanofibers containing metal–organic frameworks and Cu_2O nanoparticles: particulate matter capture and antibacterial activity

Sungwoo Jung, Kang Hyun Park*

Department of Chemistry, Pusan National University, Korea

Protection from particulate matter (PM10 and PM2.5) and microorganisms using MOFs (metal–organic frameworks) and nanoparticles used in filtration has been a major challenge. In this study, poly(vinylidene fluoride) (PVDF) nanofibers embedded with MOF-801 and Cu_2O nanoparticles were prepared using electrospinning. The modified nanofibers adsorb particulate matter (PM10 and PM2.5) and reduce microorganism populations, thereby improving filtration and antibacterial processes. The multifunctional nanomaterials, which are suitable for use in the presence of hazardous concentrations of particulate matter and E. coli because of the well-dispersed MOF-801 and Cu_2O on the nanofibers, show very efficient particulate matter adsorption (PM2.5: 64.46%, PM10: 63.19% after 5 min and PM2.5: 88.26%, PM10: 85.22% after 10 min, respectively).



Poster Presentation : **INOR.P-10**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

[Withdrawal] Fluorescent-turn off chemosensor based on sulfonamide for detecting Hg^{2+}

Kim Gyeongjin, **Donghwan Choe**[1], **Jiyoung Lee**[2], **Cheal Kim**[2,*]

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

[1]*Seoul National University of Science & Technology, Korea*

[2]*Fine chemistry, Seoul National University of Science & Technology, Korea*

- Withdrawal -

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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

[Withdrawal] A novel fluorescent turn-on probe based on thiosemicarbazide-naphthalene for selectively detecting Zn^{2+}

Minji Lee, Hyeongjin Kim, Cheal Kim*

Fine Chemistry, Seoul National University of Science & Technology, Korea

Poster Presentation : **INOR.P-12**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

The transition from Heterogeneous metals to Homogeneous metals in Metal–Organic Frameworks

Jung Heum Yoon, Giseong Lee[1], Woo Ram Lee[2,*]

Department of Chemistry, Hallym University, Korea
[1]Department of Chemistry, Kookmin University, Korea
[2]School of Future Convergence, Department of Chemistry and Institute of Applied Chemistry, Korea

Two novel heterometallic organic frameworks, LnZnTPO **1** and **2** and two homometallic MOFs, LnTPO **3** and **4** (Ln = Eu for **1** and **3**, Tb for **2** and **4**; H_3TPO = tris-(4-carboxyphenyl)phosphine oxide) were synthesized, which were prepared by solvothermal reaction of C_3 symmetric ligand H_3TPO and the corresponding metal ion(s) (a mixture of Ln^{3+} and Zn^{2+} for **1** and **2**, and Ln^{3+} alone for **3** and **4**). As a result of single crystal X-ray diffraction (SXRD) analysis, **1** and **3** were found to have conformal structures as **2** and **4**. Thermogravimetric analysis (TGA) showed that the framework is thermally stable up to about 400 °C for **1** and **2**, and about 450 °C for **3** and **4**. Powder X-ray diffraction (PXRD) analysis showed a change in the pore structure during the drying process. The forms of gas sorption isotherms for **1** and **3** are almost identical to those for **2** and **4**, respectively. Solvothermal immersion of **1** and **2** in Tb^{3+} and Eu^{3+} solutions resulted in the framework metal-ion exchange affording **4** and **3** , respectively, as confirmed by photoluminescence (PL), PXRD, infrared (IR), and inductively coupled plasma atomic emission spectroscopy (ICP-AES) analyses.

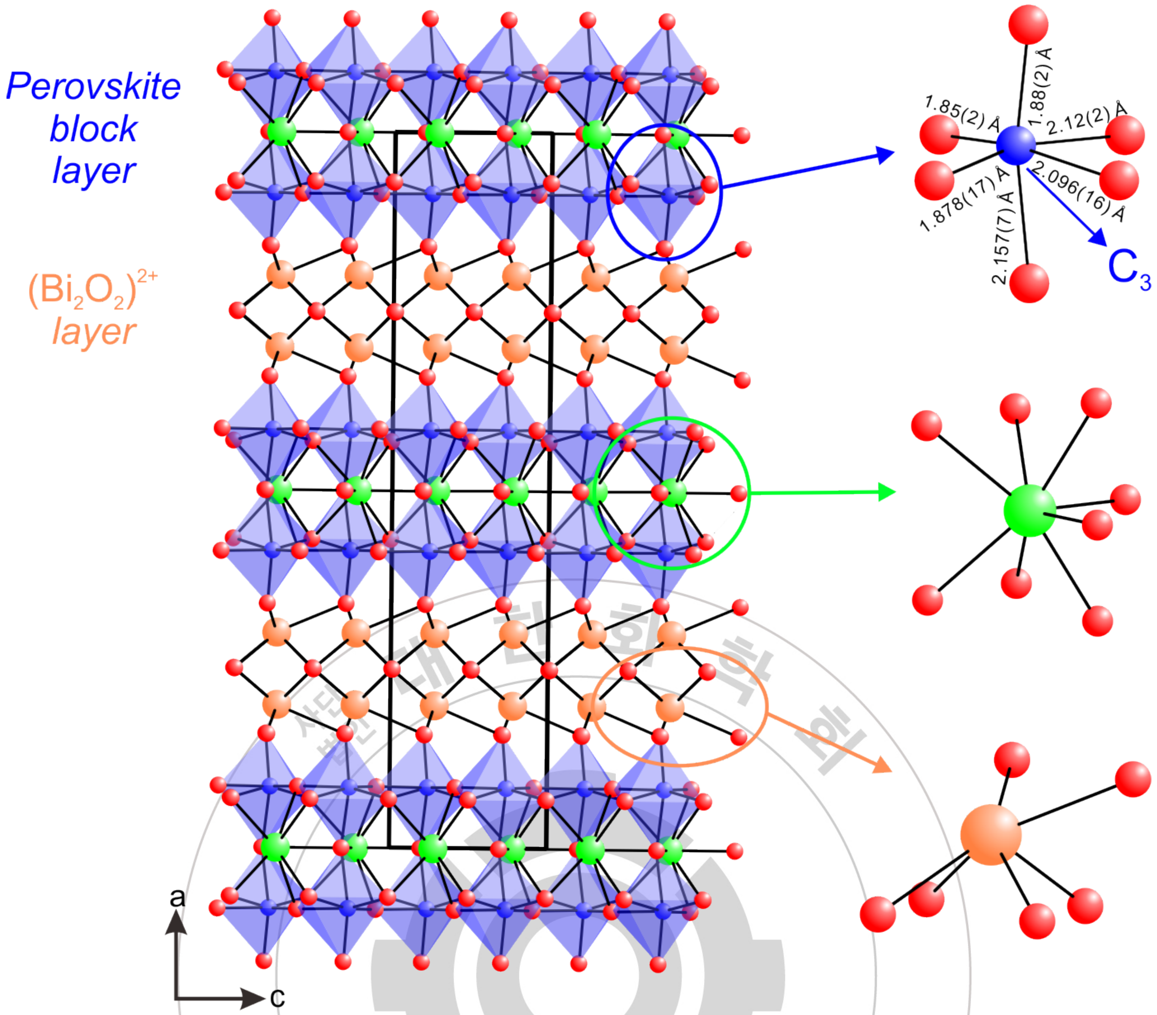
Poster Presentation : **INOR.P-13**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Nonlinear Optical Properties of Rare-Earth Metal-Doped Layered Perovskites, $Na_{0.45}Bi_{2.5}RE_{0.05}Nb_2O_9$ (RE = Eu, Sm, and Pr)

Kisung Kim, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Perovskites, one of the most interesting subjects in many research areas with a variety of characteristics such as ferroelectricity, pyroelectricity, piezoelectricity, and heterogeneous catalytic activity have been of great interest. Among them, a layered perovskite, $Na_{0.45}Bi_{2.5}RE_{0.05}Nb_2O_9$, consisting of two families of second-order Jahn–Teller distortive cations, namely, the lone pair cation, Bi^{3+}, and the octahedrally coordinated d^0 transition metal cation, Nb^{5+}, with macroscopic noncentrosymmetric structure has been studied for its ferroelectricity and piezoelectricity. We have focused on the nonlinear optical (NLO) properties of $Na_{0.45}Bi_{2.5}RE_{0.05}Nb_2O_9$ and redetermined the crystal structure by single crystal X-ray diffraction. We found a great difference of the NLO properties after substituting lone pair cations with some of rare earth elements. The origin of great NLO properties of $Na_{0.45}Bi_{2.5}RE_{0.05}Nb_2O_9$ is explained in detail using the difference. Electron localized function diagram, total and partial density of states, and band structure calculations for $Na_{0.45}Bi_{2.5}RE_{0.05}Nb_2O_9$ also support the explanation.


Perovskite block layer
$(Bi_2O_2)^{2+}$ layer
1.85(2) Å
1.88(2) Å
2.12(2) Å
1.878(17) Å
2.096(16) Å
2.157(7) Å
C_3
a
c

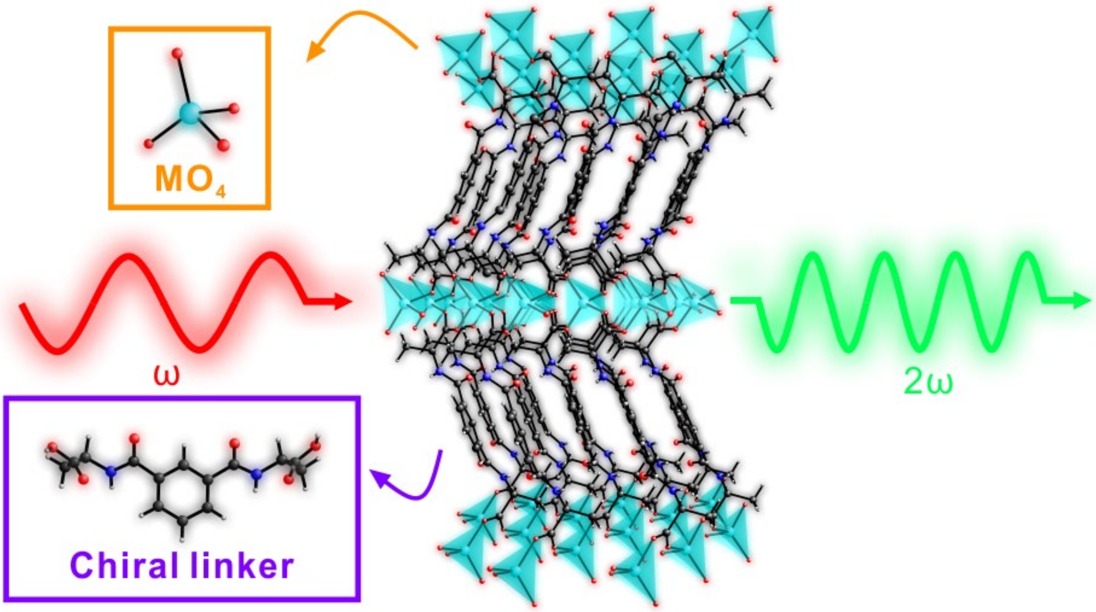
Poster Presentation : **INOR.P-14**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Chiral Zn- and Cd-coordination polymers with very strong second-harmonic generation

Joonhyuk Kee, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Novel chiral coordination polymers (CPs), M(*S*) and M(*R*) (M = Zn, Cd), have been successfully synthesized by hydrothermal reactions with the designed chiral ligands. M(*S*) and M(*R*) crystallizing in the nonpolar space group, $C222_1$, reveal three-dimensional structure consisting of MO_4 tetrahedra connected by the introduced chiral organic ligands. Ultraviolet-visible diffuse reflectance spectra reveal that the band gaps of the title compounds are *ca*. 4.15 eV. Solid-state circular dichroism spectra reveal peaks with the opposite direction at 223 and 260 nm owing to the Cotton effect. Powder second-harmonic generation (SHG) measurements indicate that Zn(*S*), Zn(*R*), Cd(*S*), and Cd(*R*) reveal SHG efficiency of *ca*. 5–9 times that of KH_2PO_4. The large SHG efficiency may come from the strong donor–acceptor system with a large hyperpolarizability.



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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis, structure, and magnetic properties of a hexanuclear iron(III) complex

Hyejin Shin, Inseong Jung, Kil Sik Min[1,*]

Chemistry Education, Kyungpook National University, Korea

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

Hexanuclear iron complex, [(pmidp)2Fe6(CH3O)4(N3)4(CH3OO2)O2] (1), has been prepared by the reaction of N-(2-pyridylmethyl)iminodipropanol (H2pmidp), NaN3, and Fe(OAc)2 in methanol/acetonitrile. The complex was characterized by elemental analysis, IR and UV/vis spectroscopies as well as single crystal X-ray diffraction. The complex crystallized in the monoclinic P21/n space group. All iron ions in 1 show 6-coordinated geometric structure. To confirm the oxidation states of iron ions we have investigated via Mössbauer spectrum and bond valence sum calculations. Therefore, we have demonstrated that the oxidation states of iron ions are all 3+. In addition, we have studied magnetic interactions to display antiferromagnetic and ferromagnetic couplings using MPMS data. In this poster, we will present and discuss the synthesis, structure, and physical properties of the iron(III) complex.

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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis, Crystal Structure, and Characterizations of Polar d^{10} Metal Coordination Compounds

Woo young Seo, Kang Min Ok[*]

Department of Chemistry, Sogang University, Korea

Using a slow evaporation method, four novel chiral d^{10} metal coordination compounds were successfully synthesized. Single crystal X-ray diffraction shows that zinc and cadmium compounds crystallize in the polar monoclinic space group, $P2_1$ and triclinic space group, $P1$, respectively. While distorted $ZnBr_3O$ tetrahedra are formed through the coordination of one O atom and three Br atoms to zinc in Zn compounds, distorted $CdOCl_4$ trigonal bipyramids are formed via connections of one O atom and four Cl atoms to cadmium in Cd compounds. In Zn and Cd compounds, each compound has pseudo 1D and 3D structures, respectively, by hydrogen bonding interactions. Local dipole moment calculations indicate the alignment of polyhedra results in a net polarization in each compound. Further characterizations, including powder X-ray diffraction and powder second–harmonic generation (SHG) measurements are also presented.

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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Polar Niobium Oxyfluorides and Tantalum Fluorides Templated by Chiral Histidinium Cations

Heejung Choi, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Polar hybrid compounds with macroscopic NCS structures were successfully synthesized by using enantiopure histidine and niobium or tantalum cations as asymmetric building units through slow evaporation reactions under acidic media. Single crystal X-ray diffraction indicates that all the title compounds crystallize in the polar space group, $P2_1$. Hydrogen bonds between polyhedra of niobium or tantalum cations and histidine have the title compounds to crystallize in pseudo-three dimensional structures. While partial density of states for Nb compounds indicate that O atoms of inorganic units mainly contribute to the conduction band (CB) and valence band (VB), those of Ta compounds reveal that CB and VB are mainly composed of C atoms of histidinium. Opposite circular dichroism signals confirm that all the reported compounds are chiral. Second harmonic generation (SHG) measurements indicate that the title compounds are type-I phase-matchable with SHG efficiency of 0.5 times that of KH_2PO_4.

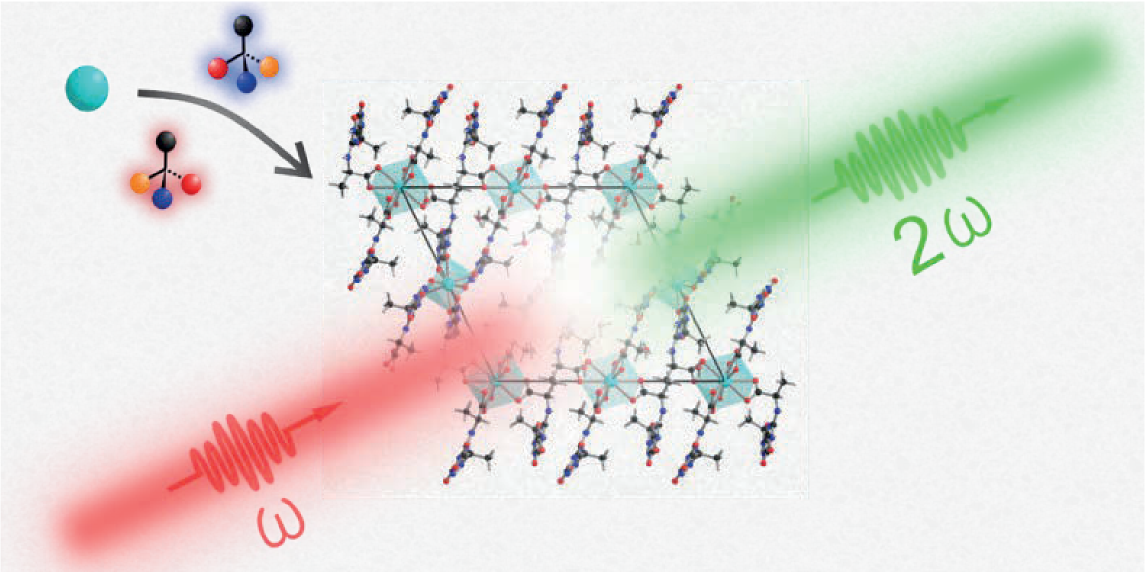
Poster Presentation : **INOR.P-18**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Novel enantiomorphic lanthanide-based coordination polymers with optical properties

Yunseung Kuk, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Coordination polymers (CPs) have been of great interest owing to their intriguing properties such as selective host-guest interactions with framework flexibility, selective separations with adjustable pore sizes, and catalytic activities with open metal sites. Especially, introducing chirality into CPs may form a novel framework toward the macroscopic noncentrosymmetric (NCS) structures, resulting in useful properties such as second-harmonic generation (SHG), ferroelectricity, piezoelectricity, pyroelectricity, and chiral properties. However, the preparation of CPs with NCS structures is a highly challenging task because most of solid-state materials prefer to crystallize in thermodynamically stable centrosymmetric structures. In order to prepare CPs with macroscopic NCS structures more systematically, novel chiral organic ligands were carefully designed and synthesized. By introducing the chiral linkers, enantiomorphic lanthanide-based coordination polymers have been successfully synthesized through solvothermal reactions. The title compounds not only absorb circularly polarized light, but also reveal SHG signals originating from the macroscopic NCS structures. The reported chiral CPs are further characterized by spectroscopic, thermal, and elemental analyses.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Poster Presentation : **INOR.P-19**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis, Structures and Characterizations of homochiral coordination polymers constructed from a V-shaped Alanine derivative

Jihyun Lee, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Two homochiral metal-organic coordination polymers (CPs) have been hydrothermally synthesized by using V-shaped alanine derivative chiral ligands. The title compounds with three-dimensional (3D) frameworks crystallized in the triclinic space group, $P1$ with 5- and 6-coordinated Zn^{2+} cations and 6-coordinated Cd^{2+} cations, respectively. While two chiral ligands, L^{2-}, were coordinated to metal cations along the equatorial positions, bipy ligands were connected along the axial direction. Thermogravimetric analysis indicates that the reported CPs have good thermal stabilities up to 350 °C. Ultraviolet-visible diffuse reflectance spectra reveal that the title compounds have approximate band gaps of 3.8 eV. Powder second–harmonic generation (SHG) measurements indicate that the reported compounds have SHG efficiencies of ca. 0.5-1.1 times that of KH_2PO_4.

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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

New noncentrosymmetric niobium oxyfluorides templated by synthetic chiral amino acids

<u>Jihyeon Moon</u>, Kang Min Ok[*]

Department of Chemistry, Sogang University, Korea

Chiral niobium oxyflourides have been synthesized by hydrothermal reactions with the aid of enantiomorphic synthetic amino acids, 4-hydroxy-D-(-)-2-phenylglycine and 4-hydroxy-L-(+)-2-phenylglycine. Large-sized colorless crystals of title materials were grown by a slow evaporation method in a dry condition. Single-crystal X-ray diffraction suggests that the reported compounds crystallize in the noncentrosymmetric nonpolar space group, $P2_12_12$. The molecular structures are composed of cationic chiral amino acids and anionic $[NbOF_5]^{2-}$ distorted octahedra. Hydrogen bonding interactions between N-H or O-H groups in organic cations and O or F atoms in $[NbOF_5]^{2-}$ octahedra occur in the structure. The adjacent benzene rings in chiral amino acids also interact with $[NbOF_5]^{2-}$ octahedra through π-π interactions. A large crystal of the title compound polished along the (021) plane exhibits a large birefringence. Thermal properties, various spectroscopic analyses, and powder second-harmonic generation properties along with electronic structure calculations are provided.

Poster Presentation : **INOR.P-21**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Impact of sphingosine and acetylsphingosines on the aggregation and toxicity of metal-free and metal-treated amyloid-β

Yelim Yi, Mi Hee Lim*

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

Pathophysiological shifts in the cerebral levels of sphingolipids in Alzheimer's disease (AD) patients suggest a link between sphingolipid metabolism and the disease pathology. Sphingosine (**SP**), a structural backbone of sphingolipids, is an amphiphilic molecule that is able to undergo aggregation into micelles and micellar aggregates. Considering its structural properties and cellular localization, we hypothesized that **SP** potentially interacts with amyloid-β (Aβ) and metal ions that are found as pathological components in AD-affected brains, with manifesting its reactivity towards metal-free Aβ and metal-bound Aβ (metal–Aβ). In this presentation, we will report that **SP** is capable of interacting with both Aβ and metal ions and consequently affects the aggregation of metal-free Aβ and metal–Aβ. Moreover, incubation of **SP** with Aβ in the absence and presence of metal ions results in the aggravation of toxicity induced by metal-free Aβ and metal–Aβ in living cells. As the simplest acyl derivatives of **SP**, N-acetylsphingosine and 3-O-acetylsphingosine also influence metal-free Aβ and metal–Aβ aggregation to different degrees, compared to **SP**. Such slight structural modifications of **SP** neutralize its ability to exacerbate the cytotoxicity triggered by metal-free Aβ and metal–Aβ. Notably, the reactivity of **SP** and the acetylsphingosines towards metal-free Aβ and metal–Aβ is determined to be dependent on their formation of micelles and micellar aggregates. Our overall studies demonstrate that **SP** and its derivatives could directly interact with pathological factors in AD and modify their pathogenic properties at concentrations below and above critical aggregation concentrations.[1]

Reference

1. Y. Yi, Y. Lin, J. Han, H. J. Lee, N. Park, G. Nam, Y. S. Park, Y.-H. Lee, M. H. Lim, *Chem. Sci.* **2021**, *12*, 2456–2466.

Poster Presentation : **INOR.P-22**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Photocatalytic Hydrogen Evolution from Plastoquinol Analogues with a Cobalt Complex and an Organic Photoredox Catalyst as a Photosystem I Functional Model

Young Hyun Hong, Yong-Min Lee[1], Shunichi Fukuzumi[2,*], Wonwoo Nam[*]

Department of Chemistry and Nano Science, Ewha Womans University, Korea
[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*
[2]*Faculty of Science and Engineering, Meijo University, Japan*

The recent development of a functional model of photosystem II (PSII) has paved a new way to connect the PSII model with a functional model of photosystem I (PSI). However, PSI functional models have yet to be reported. We report herein the first potential functional model of PSI, in which plastoquinol analogues were oxidized to plastoquinone analogues, accompanied by hydrogen evolution. Photoirradiation of a deaerated acetonitrile solution containing hydroquinone derivatives (X-QH_2) as a hydrogen source, 9-mesityl-10-methylacridinium ion (Acr^+-Mes) as a photoredox catalyst, and a cobalt(III) complex, $Co^{III}(dmgH)_2pyCl$ as a redox catalyst resulted in the evolution of H_2 and formation of the corresponding *p*-benzoquinone derivatives (X-Q) quantitatively. Photocatalytic H_2 evolution is started by electron transfer (ET) from Cl_4QH_2 to the triplet ET state of Acr^+-Mes to produce $Cl_4QH_2^{\bullet +}$ and $Acr^{\bullet}$-Mes with a rate constant of 7.2×10^7 M^{-1} s^{-1}, followed by ET from $Acr^{\bullet}$-Mes to $Co^{III}(dmgH)_2pyCl$ to produce $[Co^{II}(dmgH)_2pyCl]^-$, accompanied by the regeneration of Acr^+-Mes. On the other hand, $Cl_4QH_2^{\bullet +}$ is deprotonated to produce $Cl_4QH^{\bullet}$, which transfers either a hydrogen-atom transfer or a proton-coupled electron transfer to $[Co^{II}(dmgH)_2pyCl]^-$ to produce a cobalt(III) hydride complex, $[Co^{III}(H)(dmgH)_2pyCl]^-$, which reacts with H^+ to evolve H_2, accompanied by the regeneration of $Co^{III}(dmgH)_2pyCl$. The formation of $[Co^{II}(dmgH)_2pyCl]^-$ was detected by electron paramagnetic resonance measurements. (Reference: Hong, Y. H.; Lee, Y.-M.; Nam, W.; Fukuzumi, S. *Inorg. Chem.* **2020**, *59*, 14838-14846.)

Poster Presentation : **INOR.P-23**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Unprecedented High O-O Stretch and Electrophilic Reactivity of a Mononuclear Nonheme Iron(III)-Peroxo Complex

Semin Jang, Yong-Min Lee[1], Mi Sook Seo[2], Wonwoo Nam[3,*]

Ewha Womans University, Korea
[1]*Research Institute for Basic Sciences, Ewha Womans University, Korea*
[2]*Institute of Nano & BioTechnology, Ewha Womans University, Korea*
[3]*Department of Chemistry and Nano Science, Ewha Womans University, Korea*

A mononuclear nonheme iron(III)-peroxo complex, $[Fe(III)(O_2)(13\text{-}TMC)]^+$ (**1**), was synthesized and characterized spectroscopically; the characterization with EPR, Mössbauer, XAS, mass, and resonance Raman spectroscopies supported a high-spin $S = 5/2$ Fe(III) species binding an O_2-unit. A notable observation was an unusually high $\upsilon_{O\text{-}O}$ at ~1000 cm^{-1} for the peroxo ligand. In reactivities, **1** showed an electrophilic reactivity in hydrogen atom (H-atom) abstraction and oxygen atom transfer (OAT) reactions. In the H-atom reaction, a kinetic isotope effect (KIE) value of 5.8 was obtained in the oxidation of 9,10-dihydroanthracene. In the OAT reaction, a negative ρ value of –0.61 in Hammett plot was determined in the oxidation of *para*-X-substituted thioanisoles. Another interesting observation was the electrophilic reactivity of **1** in the oxidation of benzaldehyde derivatives, such as a negative ρ value of –0.77 in Hammett plot and a KIE value of 2.2. To the best of our knowledge, the present study reports the first example of a mononuclear nonheme iron(III)-peroxo complex with an unusually high $\upsilon_{O\text{-}O}$ value and an unprecedented electrophilic reactivity in oxidation reactions.

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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Dioxygen Activation at Mn(III) Corrole Center: Reversible O-O Bond Formation and Cleavage

Ranjana Gupta, **Mian Guo[1]**, **Yong-Min Lee[2]**, **Mi Sook Seo[3]**, **Shunichi Fukuzumi[4,*]**, **Wonwoo Nam[*]**

Department of Chemistry and Nano Science, Ewha Womans University, Korea
[1]*College of Chemistry and Molecular Sciences, Wuhan University, China*
[2]*Research Institute for Basic Sciences, Ewha Womans University, Korea*
[3]*Institute of Nano & BioTechnology, Ewha Womans University, Korea*
[4]*Faculty of Science and Engineering, Meijo University, Japan*

We report the O_2-activation and O-O bond formation reactions by manganese(III) corrole complexes. In the O_2-activation reactions, the formation of Mn(V)-oxo (**1**) and Mn(IV)-peroxo (**2**) intermediates was observed when Mn(III) corrole complexes were exposed to O_2 in the presence of base (*e.g.*, OH^-) and hydrogen atom (H-atom) donors (*e.g.*, THF or cyclic olefins). The Mn(V)-oxo and Mn(IV)-peroxo intermediates were fully characterized spectroscopically by synthesizing authentic compounds. In the O-O bond formation reactions, addition of hydroxide ion to the Mn(V)-oxo species afforded the Mn(IV)-peroxo species, and the O-O bond formation and cleavage reactions between the Mn(V)-oxo and Mn(IV)-peroxo complexes were reversible. The role of base was proposed to lower the oxidation potentials of the Mn(III) corroles, leading to binding of O_2 and forming Mn(IV)-superoxo species. This putative Mn(IV)-superoxo species was then converted to the corresponding Mn(IV)-hydroperoxo species by H-atom abstraction from H-atom donors, followed by the O-O bond cleavage of the putative Mn(IV)-hydroperoxo species to form Mn(V)-oxo. In contrast, Mn(IV)-peroxo was formed as the final product in the presence of an excess amount of base. To the best of our knowledge, the present study reports the first example of using the same manganese complex in both O_2-activation and O-O bond formation reactions.

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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Novel Palladium(II) Complexes with *N*-Substituted *N,N′*-Aminomethylquinolines and *N,N′*-Aminomethylpyridines: Synthesis, Structures, and Polymerization of Cyclic Olefins

Ahrim Jeong, Hyosun Lee[*]

Department of Chemistry, Kyungpook National University, Korea

New palladium(II) mononuclear complexes, namely, **[(L_A)$PdCl_2$] (1)**, **[(L_B)$PdCl_2$] (2)** and **[(L_C)$PdCl_2$] (3)**, have prepared by using [$Pd(MeCN)_2Cl_2$] with *N, N'*-bidentate ligands L_n [L_n = L_A-L_C; L_A = 4-(pyridine-2-ylmethyl)morpholine, L_B = 4-(quinolin-2-ylmethyl)morpholine, L_C = 2-(piperidin-1-ylmethyl)quinolone]. All complexes were characterized by ^1H NMR, ^{13}C NMR, FT-IR, elemental analysis, and SC-XRD. In all complexes, Pd(II) ion is coordinated with two nitrogen atoms from L_n (L_n = L_A, L_B and L_C) ligand and two Cl atoms, thus, exhibited a distorted square planar geometry. These palladium(II) complexes show catalytic activity for the polymerization of norbornene (NBE) and norbornene derivatives in the presence of MMAO. Furthermore, all complexes also exhibit catalytic activity toward polymerization of methyl methacrylate(MMA) in the presence of MMAO.

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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Cobalt(II) Complexes Containing *N*-Substituted 2-Iminomethylpyridine and 2-Iminomethylquinoline: Synthesis, Structure and Polymerization of Norbornene and Norbornene Derivatives

Kyeonghun Kim, Hyosun Lee[*]

Department of Chemistry, Kyungpook National University, Korea

We have synthesized series of Co(II) complexes containing ligands **L_A**, **L_B** and **L_C** where **L_A** is (*E*)-3-methoxy-*N*-(quinolin-2-ylmethylene)propan-1-amine, **L_B** is (*E*)-N^1,N^1-dimethyl-N^2-(pyridin-2-ylmethylene)ethane-1,2-diamine and **L_C** (*E*)-*N*-(quinolin-2-ylmethylene)hexan-1-amine. All complexes were characterized by IR and elemental analyzer, and X-ray single crystal diffraction. Specifically, **[L_ACoCl_2]** adopted distorted trigonal bipyramidal geometry around metal center, however, **[L_CCoCl_2]** adopted distorted square tetrahedral geometry around cobalt metal center. The catalytic properties of these complexes toward the polymerization of norbornene (NBE) and norbornene derivatives in the presence of modified methylaluminoxane (MMAO) were also investigated. The catalytic experiments were performed by changing the temperature, polymerization time, and amount of precatalyst and co-catalyst for optimizing the polymerization of cyclic olefins.

Poster Presentation : **INOR.P-27**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Zinc(II) Complexes with *N*-Substituted *N*,*N'*-Aminomethylquinoline and *N*,*N'*-Aminomethylpyridine Derived Ligands: Synthesis, Structural Characterization and *rac*-Lactide Polymerization

Jaegyeong Lee, **Hyosun Lee***

Department of Chemistry, Kyungpook National University, Korea

New series of zinc(II) complexes were synthesized by the reaction of ligands L_n [$L_n = L_A – L_D$; L_A = 2-(piperidin-1-ylmethyl)quinoline, L_B = 4-(quinolin-2-ylmethyl)morpholine, L_C = 4-(pyridin-2-ylmethyl)morpholine and L_D = 2-(piperidin-1-ylmethyl)pyridine], and metal starting material **[ZnCl2]** in ethanol at room temperature. Each complex was characterized by ^{1}H-NMR, ^{13}C-NMR, IR, elemental analyzer, and single crystal X-ray diffraction. The catalytic properties of these complexes toward the polymerization of *rac*-lactide (LA) in the presence of Me_2CHOLi were investigated at three different temperatures, 25 °C, 0 °C and -25 °C.

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

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis, Characterization and Polymerization of *rac*-Lactide by Copper(II) Complexes Containing *N*,*N'*-Bidentate Aminomethylquinolines and Aminomethylpyridines

Yerim Cho, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

We have synthesized a new series of Cu(II) complexes with ligands L_n [$L_n = L_A – L_D$; L_A is 2-(piperidin-1-ylmethyl)quinoline, L_B = 4-(quinolin-2-ylmethyl)morpholine, L_C = 4-(pyridin-2-ylmethyl)morpholine and L_D = 2-(piperidin-1-ylmethyl)pyridine]. All synthesized complexes were analyzed by various spectroscopic methods such as IR, elemental analyzer and single crystal X-ray diffraction. Specifically, molecular structure of **[L_BCuCl_2]** exhibited 4-coordinate distorted tetrahedral geometry around metal center. The catalytic properties of these complexes toward the polymerization of *rac*-lactide (LA) in the presence of Me_2CHOLi or MeLi was investigated at three different temperatures.

Poster Presentation : **INOR.P-29**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Intriguing ‘turn-on’ emissive feature of carbazole-based *o*-carboranyl luminophore via deboronation reaction

Seok Ho Lee, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

The conversion of *closo*-*o*-carborane–containing compounds to the *nido*-*o*-species via deboronation causes photophysical changes. 9-Methyl-9*H*-carbazole–based *closo*- (*closo*-**Cz**) and *nido*-*o*-carboranyl (*nido*-**Cz**) compounds were prepared and fully characterised by multinuclear NMR spectroscopy and elemental analysis, and the solid-state molecular structure of *closo*-**Cz** was analysed by X-ray crystallography. *Nido*-**Cz** showed a distinct emission band in THF at 298K centered at λ_{em} = ca. 380 nm, which was attributed to an intramolecular charge transfer (ICT) transition because *nido*-*o*-carborane is an electronic donor, whereas *closo*-**Cz** did not exhibit any emissive trace. The positive solvatochromic effect of *nido*-**Cz** and the results of theoretical calculations for both the *o*-carboranyl compounds supported that these emissive features originate from ICT corresponding to the *o*-carborane. Furthermore, the calculations verified that the electronic role of the *o*-carboranyl unit changed from acceptor to donor upon deboronation from *closo*-**Cz** to *nido*-**Cz**. Investigations of the radiative decay mechanisms of *closo*-**Cz** and *nido*-**Cz** according to their quantum efficiencies (Φ_{em}) and decay lifetimes (τ_{obs}) suggested that the ICT-based radiative decays of *closo*-**Cz** and *nido*-**Cz** readily occur in the film (solid) and solution state, respectively. These observations suggested that the emission intensity of *closo*-**Cz** in the solution state could be drastically enhanced by deboronation to *nido*-**Cz** upon exposure to an increasing concentration of fluoride anions. Indeed, turn-on emissive features in an aqueous solution were observed upon deboronation. All these findings strongly indicate that *closo*-**Cz** has the potential for use as a turn-on and visually detectable chemodosimeter for fluoride ion sensing.

Poster Presentation : **INOR.P-30**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Molecular Design of Fluorene based *closo-ortho*-Carboranyl Luminophores Manifesting Thermally Activated Delayed Fluorescence

Dong Kyun You, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

We propose a strategic molecular design of *closo-o*-carborane-based donor–acceptor dyad system that exhibits thermally activated delayed fluorescence (TADF) in solution state at ambient temperature. Planar 9,9-dimethyl-9*H*-fluorene-based compounds with *closo*- and *nido-o*-carborane cages appended at the C2-, C3-, and C4-positions of each fluorene moiety(*closo*-type: **2FC**, **3FC**, **4FC**, and **4FCH**, and *nido*-type: *nido*-**4FC** = [*nido*-form of **4FC**]·[NBu_4]) were prepared and characterized. The crystal structure of **4FC** exhibited a significantly distorted fluorene plane, which revealed a severely intramolecular steric hindrance. Interestingly, **4FC** demonstrated intense ICT-based emission in all states(solution at 298 K and 77 K, film, and aggregated states), while other *closo*-compounds demonstrated emissions in only the rigid state. Relative energy barriers and dihedral angles around *o*-carborane cages changed in *closo*-compounds, which indicated that *o*-carborane cages in the compounds except for **4FC** could be freely rotated at ambient temperature, whereas the structural formation of **4FC** was fixed around its S_0-optimized structure. Further, the **4FC** demonstrated that separated PL decay components were short-lived (~0.5 ns) and long-lived (27–39 ns) in the solution at 298 K and in the film state, respectively, which could be attributed to the prompt fluorescence and TADF, respectively. Such a characteristic for **4FC** was revealed by maintaining the significantly small ΔE_{ST} in the structural fixation. Consequently, the strategical molecular design of the *o*-carborane-appended π-conjugated (D–A) system, which can form rigid structural geometries, can enhance radiative efficiency for ICT-based emission and trigger intriguing photophysical properties such as the TADF nature.

Poster Presentation : **INOR.P-31**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Relationship between Electronic Effect and Intramolecular-Charge-Transfer-Based Radiative Decay Efficiency in *o*-Carboranyl Carbazole Compounds

Sehee Im, Kang Mun Lee[*]

Department of Chemistry, Kangwon National University, Korea

We report the preparation and characterization of four 9*H*-carbazoles bearing *o*-carborane units appended to the C1-C4 positions of the carbazole rings (compounds **C1**-**C4**). The impact of the electronic effect of the carbazole group on the radiative decay process based on the intramolecular charge transfer (ICT) transition of *closo*-*o*-carborane was examined herein. Although none of the *o*-carboranyl compounds exhibited emission in the solution state at 298 K, intense emissions in the region of λ_{em} = 530–600 nm were broadly observed in the rigid state. Theoretical calculations on the first excited (S_1) state indicated that the emission could be distinctly attributable to ICT transitions between the *o*-carborane and carbazole groups. Photoluminescence experiments of the compounds in THF-water mixtures also confirmed the aggregation induced emission phenomenon. Interestingly, **C1** and **C3** exhibited significantly higher quantum yields (Φ_{em}) and radiative decay constants (k_r) in the film state than **C2** and **C4**, indicating more efficient ICT-based radiative decay for **C1** and **C3**, where the *o*-carborane cage is appended to *ortho*- and *para*- positions (C1- and C3-positions) of the carbazole group. In addition, energy barrier calculations for the various compounds revealed that such differences in the emission characteristics were unrelated to the structural variation effect. Consequently, the results of this study confirm the electronic effect of the carbazole moiety in that the anionic character of the carbon atom attached to the *o*-carborane unit can reinforce the radiative decay process based on ICT transitions.

Poster Presentation : **INOR.P-32**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Strategic Molecular Design of *o*-Carboranyl-Anthracene-Dyads to Enhance Intramolecular-Charge-Transfer-Based Emission

Ju Hyun Hong, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Four phenylanthracene-based *o*-carboranyl compounds with phenyl (**AC**) and biphenyl rings (***o*AC**, ***m*AC** and ***p*AC**) appended at C10 were prepared and fully characterized to establish a design strategy for enhancing the solution- and solid-state emissive properties of *closo*-*o*-carboranyl luminophores at ambient temperature. In all solid-state molecular structures, the anthracene moieties were severely distorted because of intramolecular steric hindrance, which indicated that structural variation around the *o*-carborane cage was strongly inhibited. Compared to the other *o*-carboranyl compounds, ***o*AC**, possessing an *ortho*-type biphenyl group, exhibited much higher emission intensity, quantum efficiency, and radiative decay constant in tetrahydrofuran solution and film state at 298 K. The ground-state energy barriers were calculated based on the relative energies at dihedral angles centered at the bonding axis between anthracene and (bi)phenyl groups. These findings verify that the rotational motion of the C10-(bi)phenyl rings in ***o*AC** was more effectively restricted than in the other compounds. Furthermore, the orbital contributions calculated for electronic transitions in the first excited state indicated that structural variation around the terminal (bi)phenyl rings prevented efficient ICT transitions. Thus, the introduction of additional rigid substituents into the parent scaffold of the *o*-carboranyl luminophore enhanced the efficiency of the ICT-based radiative process. These findings provide insights into the molecular design of novel *o*-carboranyl luminophores and facilitate the maximization of their emissive properties.

Poster Presentation : **INOR.P-33**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and structural characterization of chelated diphosphine-coordinatedgold(I) complexes

Heekwon Park, Yong-Joo Kim*

Department of Chemistry, Gangneung-Wonju National University, Korea

Chelated diphosphine lignads including ferrocene derivatives show a variety of coordination modes such as three or four coordination to gold atom and formation of bridging dinuclear gold complexes. In addition, the diphosphine-coordinated gold(I) complexes display Au-P linked monomeric, dimeric, and polymeric fromation of gold complexes and also inter or intramolecular Au... Au aurophilic interactions depending on the ancillary ligand. In this context, we have interested in chelated diphosphine gold complexes containing pseudohalogen ligands and their monomeric or polymeric structures which can reveal potential Au-Au interactions and be applied to dipolar cycloaddition for heterocycle formation. In this work, we have attempted to the formation of new monomeric or polymeric gold(I) complexes bridged by a ferrocenyl diphophine ligand containing pseudohalgen ligands such as CF_3COO or azido ligand. Detail explanation will be discussed.

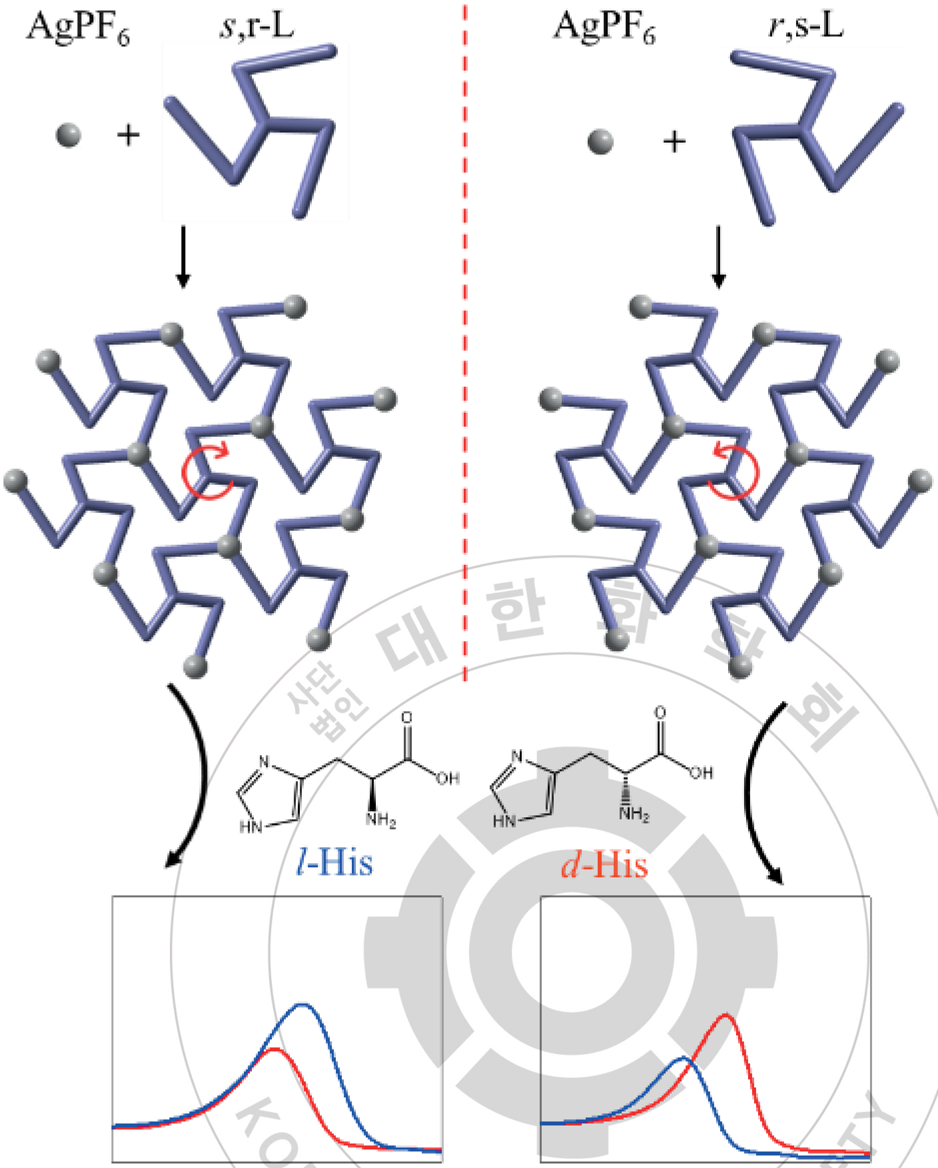
Poster Presentation : **INOR.P-34**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Pair of chiral 2D silver(I) enantiomers: recognition of chiral histidine via differential pulse voltammetry

Dongwon Kim, Ok-Sang Jung[*]

Department of Chemistry, Pusan National University, Korea

Self-assembly of $AgPF_6$ with a pair of chiral tridentate ligands, (1*S*,1'*S*,1"*S*,2*R*,2'*R*,2"*R*) and (1*R*,1'*R*,1"*R*,2*S*,2'*S*,2"*S*)-(benzenetricarbonyltris(azanediyl))tris(2,3-dihydro-1H-indene-2,1-diyl)triisonicotinate (*s*,*r*-L) and (*r*,*s*-L) in a mixture of methanol and dioxane yields 2D sheets consisting of [Ag(*s*,*r*-L)](PF_6)·$3C_4H_8O_2$ and [Ag(*r*,*s*-L)](PF_6)·$3C_4H_8O_2$, respectively. Differential pulse voltammetric (DPV) technique using the pair of chiral 2D sheet enantiomers was employed for chiral discrimination of amino acid enantiomers, and was found to be an effective tool for enantio-recognition of *l*- and *d*-histidines. Both size and binding site of amino acids are strongly depending on the electrochemical enantio-recognition via the chiral 2D sheets.


AgPF6
s,r-L
+
AgPF6
r,s-L
+
N
HN
O
OH
NH2
l-His
N
HN
O
OH
NH2
d-His

Poster Presentation : **INOR.P-35**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Significant qualifications for an efficient catechol oxidation catalyst in terms of structural perspective

Do Heon Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of $Cu(BF_4)_2$ and $Cu(ClO_4)_2$with ethyl(methyl)(3-pyridine)silane (L) as a bidentate N-donor. At the same time, $(NH_4)_2SiF_6$, NH_4PF_6, $NaSbF_6$ was added respectively. It produces new discrete cyclotrimeric rings and 4-fold interpenetrated coordination compounds. The coordination network acts as a remarkable catechol oxidation system that shows both the significant counteranion effect and coordination skeleton effect. As the coordination compound has a smaller counteranion and reacts with less dissolution in the solution phase, compounds show the higher catalytic efficiency. Efficiency of the skeleton was confirmed by varying the degree of solubility of the compound, which is conducted by controlling reaction temperature and slightly changing the composition of the acetone solvent.

Poster Presentation : **INOR.P-36**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Straightforward Formation of Acetonyl Monoanion, Dianion as Synthons: Self-assembly of Mercury(II) with Pyridyl Donor Ligands in Acetone

KangSan Hong, Ok-Sang Jung[*]

Department of Chemistry, Pusan National University, Korea

Acetone has used as one of the most important solvents in both chemical industry and laboratory. Like most ketones, acetone has known to exhibit the keto–enol tautomerism in which the nominal keto form $(CH_3)_2C=O$ of acetone itself is in equilibrium with its enol isomer $(CH_3)C(OH)=(CH2_2)$. Thus, enolates derived from the deprotonation of carbonyl compounds are widely used as reagents in the synthesis of organic compounds. Enolate anions has known to be delocalized over the oxygen and the two carbon sites, and have the character of both an alkoxide and a carbanion. Deprotonation of such enolizable ketones, aldehydes, and esters gives enolates under vigrous condition such as strong bases, lithium diisopropylamide (LDA). Some organic reactions of platinum metal complexes in acetone are accompanied by proton elimination and rearrangement of acetone molecule, which leads to the formation of various acetonyl complexes. Various M–ketonyl species have been isolated by using late-transition metals, such as Rh, Ni, Pt, Pd, and Au.[2][1][2] According to Johnson's group, mercuration occurs spontaneously, if slowly, in acidic aqueous solutions of acetone and free mercuric ion to produce at least nine organomercury species including acetonyl dianion, all of which can exist in equilibrium simultaneously.[3] To the best of our knowledge, no examples of the X-ray structure on acetonyl coordination for mercury(II) complexes has been described at all. In this context, two crucial aims of the present research were to explore stable acetonyl species via self-assembly of $Hg(ClO_4)_2$ with naphthalene-2,6 diyldipicolinate(L^1) or 1,3-bis(dimethyl(pyridin-3-yl)silyl)propane(L^2) in acetone under mild condition and to efficiently trap the acetonyl dianion species in the supramolecularr crystal for X-ray crystal-structural determination. We report proof-of-concept observations on formation and various structures of acetone enolate. This system safely shows a bridged enolate in the crystalline state along with ^1H NMR in solution.REFERENCES(1) D. Gasperini, et al. Gold–Acetonyl Complexes: From Side-Products to Valuable Synthons. Chem. Eur. J.**2015**, *21*, 5403 – 5412.(2) C. R. Barone, et al. Activation of ketones by electrophilic metal complexes: Synthesis of some ketonyl

platinum(II) complexes and X-ray crystal structure of [PtCl{$CH_2C(O)CH_3$} (1,10-phenanthroline)]·1/2Y (Y = H_2O or CH_2Cl_2). Inorg. Chim. Acta **2012**, *383*, 13–19.(3) F. A. Johnson, W. D. Perry. Mono-, Poly-, and Permercuration in the Acetone-Mercury (II) System1. Organometallics, **1989**, *8*, 2649.

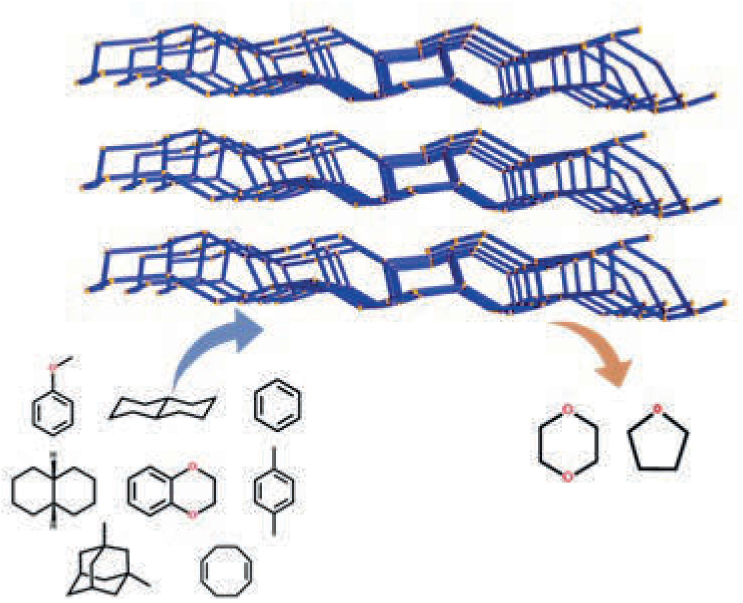
Poster Presentation : **INOR.P-37**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Comparison of guest exchanges between metal complexes in SCSC mode: various metal complexes with 2D sheet structure

Gyeongwoo Kim, Junmyeong Park, Ok-Sang Jung[*]

Department of Chemistry, Pusan National University, Korea

New ligand tri(isoquinolin-5-yl) benzene-1,3,5-tricarboxylate are synthesized by isoquinolin-5-ol . Self -assembly of $Co(NO_3)_2$, $Ni(NO_3)_2$, $Cu(NO_3)_2$, $Zn(NO_3)_2$ with L as a tridentate N-donor. They are produced of 2D sheet structures. Despite being uniquely different group metals, they have the same crystal system, space group. In this 2D sheet, the solvent is present in the sheet and also between the sheet and the sheet. In the case of all metal complexes, it was observed that most solvents including decalin and xylene became guest exchanges. However, it was confirmed that the adamantane was not exchanged for the rest of the metal complexes except for the Co complex.



128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

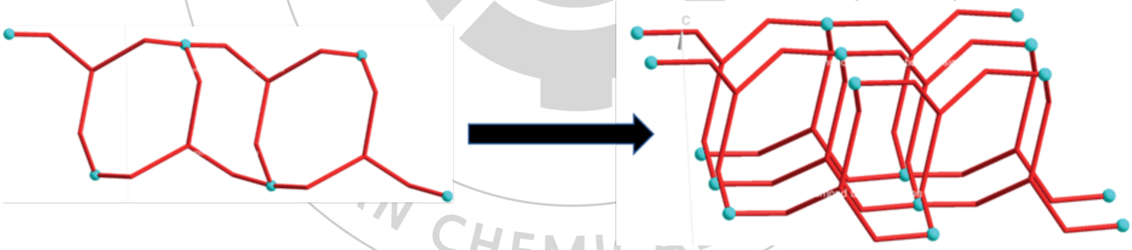
Poster Presentation : **INOR.P-38**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Dimensional change depending on solvents: 2D structure transformed from 1D in SCSC mode

Jihun Han, Seok Kyun Jeong, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self assembly of $Zn(NO_3)_2$ with 2,4,6-tris(pyridin-3-yloxy)-1,3,5-triazine (L) as a tridentate N-donor gives rise to a ladder one-dimensional (1D) structure in acetonitrile as solvent, and two-dimensional (2D) sheet structure in acetonitrile/dioxane as solvent. The 1D crystals are transformed 2D crystals mentioned above in single-crystal-to-single-crystal (SCSC) fashion by standing in the mother liquor, dioxane, for several days.



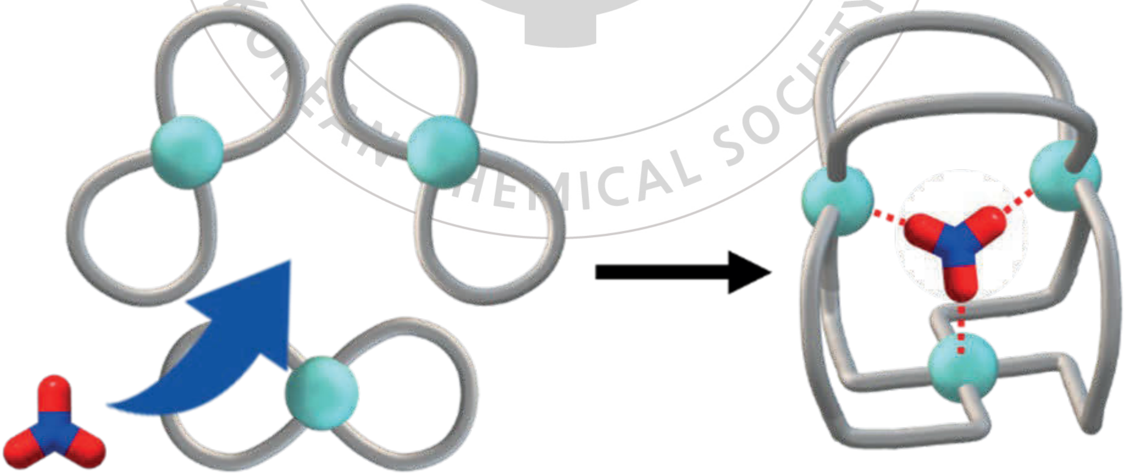
Poster Presentation : **INOR.P-39**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Formation Procedure of Trimetallic Coordination Cage for Nitrate Encapsulation

Heehun Moon, Geon Woo Gwak, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

A procedure for formation of a nitrate-encapsulating tripalladium(II) cage *via* self-assembly of $Pd(NO_3)_2$ with 1,3-bis(dimethyl(pyridin-4-yl)silyl)propane (L) was developed. The self-assembly reaction initially produces spiro-type macrocycles, PdL_2, and finally results in transformation into the nitrate-encapsulated cages, $[(NO_3)@Pd_3L_6]$, in the mother liquor. The reaction of PdX_2 ($X^- = BF_4^-$, ClO_4^-, PF_6^-, and $CF_3SO_3^-$ instead of NO_3^-) with L gives rise to the spiro species, PdL_2, as the final product, and anion exchange of the spiro products, $[PdL_2](X)_2$, with NO_3^- combines the tripalladium cages $[(NO_3)@Pd_3L_6]$.



Poster Presentation : **INOR.P-40**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Supramolecular Isomerism of Zn(II) Coordination Polymers and Their Photoreactivity

Dong Hee Lee, In-Hyeok Park*

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

Supramolecular isomers have a same chemical formula but more than one crystal structure in coordination polymers (CPs) and metal-organic frameworks (MOFs).[1] Here we demonstrate the significant correlation of solvents and coordination environments. Through solvothermal reaction of $Zn(NO_3)_2 \cdot 6H_2O$, 1,2-bis(4-pyridyl)ethylene (bpe), and 1-adamantanecarboxylicacid (Hadc), two Zn(II) supramolecular isomers are prepared under different solvent conditions based on dimethylacetamide (DMA) and dimethylformamide (DMF). A 1D zigzag CP, $[Zn(bpe)(adc)_2]$ (**1**) is synthesized from DMA which is colorless plate-shaped crystal. The mononuclear repeating unit consists of one Zn(II) atom, two bpe ligands, and two adc ligands. Zn1 atom is pseudo-tetrahedrally coordinated by two nitrogen atoms of bpe ligands and four oxygen atoms of adc ligands. On the other hand, a 1D railroad CP, $[Zn(bpe)(adc)_2]$ (**2**) is synthesized from DMF which is colorless plate-shaped crystal. The dinuclear repeating unit consists of two Zn(II) atoms, four bpe ligands, and four adc ligands. Zn1 is octahedrally coordinated by two nitrogen atoms of bpe ligands and four oxygen atoms of adc ligands. Especially, the double bonds of bpe ligands in **2** are parallelly aligned to each other at a distance of 3.6 Å. According to Schmidt's Criteria,[2] the distance between olefins within the range of 3.6-4.1 Å are photoreactive. Hence, the c=c bonds of bpe ligands in **2** undergo [2+2] cycloaddition reaction. When UV is irradiated to **2**, double bonds are converted into cyclobutane rings. The photodimerized CP $[Zn(\textit{rctt}\text{-tpcb})(adc)_2]$ (**3**, *rctt* = *regio, cis, trans, trans*; tpcb = 1,2,3,4-tetrakis(3'-carboxyphenyl)-cyclobutane) was confirmed by single crystal X-ray diffraction and ^1H nuclear magnetic resonance analyses. The details will be presented at the poster section.

References

[1] T. L. Hennigar, D. C. MacQuarrie, P. Losier, R. D. Rogers, M. J. Zaworotko, *Angew. Chem. Int. Ed. Engl.*, **1997**, *109*, 972-973.

[2] G. M. J. Schmidt, Photodimerization in the solid state, *Pure Appl. Chem.*, **1971**, *27*, 647-678.

Poster Presentation : **INOR.P-41**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Sterically Less Hindered Triazenyl Radical Stabilized by N-Heterocyclic Carbenes

Jaelim Kim, Eunsung Lee*

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

Organic radicals have great attention up to date because of their unique electronic properties and synthetic challenge. Recently, our group first reported the triazenyl radicals stabilized by the N-heterocyclic carbenes (NHCs)[1]. However, these radicals showed only single-electron transfer toward various transition-metals, and electrophiles. We proposed these limited reactivities were caused by steric hindrance nearby triazenyl cores from several types of research about radicals derived from Frustrated Lewis Pairs (FLPs)[2].Herein, we reported the triazenyl radical stabilized by the smallest NHCs. Despite weaker π-accepting properties and smaller steric effects, the introduction of the sterically less demanding NHC (IMe) to the organic radicals could support obtaining a stable redox cycle, which is attributed to that π-accepting ability of NHCs delocalizes the radical's spin density onto the carbene moiety. The detailed synthesis and full characterization of the radical including X-ray determined structure and EPR spectroscopy will be presented.Reference[1] Back, J.; Park, J.; Kim, Y.; Kang, H.; Kim, Y.; Park, M. J.; Kim, K.; Lee, E., J. Am. Chem. Soc. 2017, 139, 15300-15303.[2] Dasgupta, A.; Richards, E.; Melen, R. L., Angew. Chem. Int. Ed. 2021, 60, 53-65.

Poster Presentation : **INOR.P-42**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Minimalistic Principles for Designing Small Molecules with Multiple Reactivities against Pathological Factors in Dementia

Mingeun Kim, Mi Hee Lim[*]

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

Multiple pathogenic elements, including reactive oxygen species, amyloidogenic proteins, and metal ions, are associated with the development of neurodegenerative disorders. In this presentation, we report minimalistic redox-based principles for preparing compact aromatic compounds by derivatizing the phenylene moiety with various functional groups. These molecular agents display enhanced reactivities against multiple targets such as free radicals, metal-free amyloid-β (Aβ), and metal-bound Aβ that are implicated in the most common form of dementia, Alzheimer's disease (AD). Mechanistic studies reveal that the redox properties of these reagents are essential for their function. Specifically, they engage in oxidative reactions with metal-free and metal-bound Aβ, leading to chemical modifications of the Aβ peptides to form covalent adducts that alter the aggregation of Aβ. Moreover, the administration of the most promising candidate significantly attenuates the amyloid pathology in the brains of AD transgenic mice and improves their cognitive defects. Our studies demonstrate an efficient and effective redox-based strategy for incorporating multiple functions into simple molecular reagents.[1]Reference1.M. Kim, J. Kang, M. Lee, J. Han, G. Nam, E. Tak, M. S. Kim, H. J. Lee, E. Nam, J. Park,S. J. Oh, J.-Y. Lee, J.-Y. Lee, M.-H. Baik, M. H. Lim, *J. Am. Chem. Soc.* **2020**, *142*, 8183-8193.

Poster Presentation : **INOR.P-43**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Solvent-assisted Reversible Interpenetration of a Cu Paddlewheel-based Metal-organic Framework

Cheol Yeong Heo, Nak Cheon Jeong[*]

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

Metal-organic frameworks (MOFs), extended network consisting of metal ions (or metal-oxo clusters) and multitopic organic ligands have studied since their attractive properties such as porosity, modularity, and crystallinity. These properties give them potential functions in various fields such as gas absorption, catalysis, molecular separation, drug delivery, and sensing.MOFs with large open cavities could easily form thermodynamically stable interpenetrated framework, leading to the reducing their porosities. Although it is preferred for such applications that MOFs possess non-interpenetrated framework, interpenetrated MOFs have shown specific, selective absorption performance. So far, the control of interpenetration in MOFs and structural dynamism for MOFs have been intensively studied to achieve the desired structure. Structural transformation of MOFs could be triggered by various external stimuli such as pressure, light, heat, and guest molecules. Isolation of each single frameworks must involve the breakage of chemical bond of single framework. To the best of our knowledge, reversible structural transformation under mild condition is rarely reported.In this presentation, we show the reversible post-synthetic transformation reaction between the thermodynamically less stable non-interpenetrated framework of MOF-143 and thermodynamically more stable doubly interpenetrated framework of MOF-14. The transformation of MOF-143 to MOF-14 was preformed through the exchange of protic solvents at room temperature, whereas the reverse transformation was conducted in the presence of pyridine and DMF at100 °C. We believe that our observation and demonstration can aid in understanding the assembly and disassembly nature of framework.

Poster Presentation : **INOR.P-44**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Visible Light-driven Photochemical Conversion of CO2 by Nickel Complexes with N4S2 Coordination

Jinheung Kim[*], **Byeongmoon Jeong**[1], **Young-Mi Kim**[2]

Chemistry Department of Nano-Science, Ewha Womans University, Korea
[1]*Department of Chemistry and Nano Science, Ewha Womans University, Korea*
[2]*Chemical Engineering and Applied Chemistry, Chungnam National University, Korea*

Molecular nickel(II) complexes of pyridylbenzimidazole (pbi) and pyridylbenzothiazole (pbt) were prepared. The two Ni complexes were examined for CO2 conversion using eosin Y as a photosensitizer and triethanolamine as a sacrificial electron donor upon visible- light irradiation. Light-driven photoreduction of CO2 catalyzed by Ni(pbt)(pyS)2 and Ni(pbi)(pyS)2 (pyS = pyridine-2-thiolate) selectively affords formate with a a high efficiency and a high catalytic selectivity of ~99 %. The pbi complex exhibited a slightly faster rate and higher yield for the formate production than the pbt complex. Hydrogen production and kinetic isotope effects in the photocatalytic reactions with these Ni catalysts are also presented in relation to the CO2 reduction mechanism. These catalysts are the first examples of early transition metal complexes affording such high selectivity and efficiencies.

Poster Presentation : **INOR.P-45**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Golgi Apparatus-targeting Fluorescent Probe for the Selective Sensing of Formaldehyde

Jinheung Kim*, Sohyun Lee[1]

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

Formaldehyde (FA) is in the production of numerous household chemical goods. Here, a fluorescent chemosensor for FA is designed and prepared using a selective organ-targeting probe containing naphthalimide as a fluorophore and hydrazine as a FA-binding site. The amine group of the hydrazine reacts with FA to form a double bond and this condensation reaction is accompanied by a shift in the absorption band of the probe from 438 nm to 443 nm upon the addition of FA. Further, the addition of FA is shown to enhance the emission band at 532 nm relative to the very weak fluorescent emission of the probe itself. Moreover, a high specificity is demonstrated toward FA over other competing analytes such as calcium ion, magnesium ion, acetaldehyde, benzaldehyde, salicylaldehyde, glucose, glutathione, sodium sulfide, sodium hydrosulfide (NaHS), hydrogen peroxide, and the tert-butylhydroperoxide radical. A typical two-photon dye incorporated into the probe provides intense fluorescence upon excitation at 800 nm, thus demonstrating the potential application as a two-photon fluorescent probe for FA sensing. Furthermore, the probe is shown to exhibit a fast response time for the sensing of FA at room temperature and to facilitate intense fluorescence imaging of breast cancer cells upon exposure to FA, thus demonstrating its potential application for the monitoring of FA in living cells. Moreover, the presence of the phenylsulfonamide group allows the probe visualize dynamic changes in the targeted Golgi apparatus. Hence, the as-designed probe is expected to open up new possibilities for unique interactions with organ-specific biological molecules with potential application in early cancer cell diagnosis.

Poster Presentation : **INOR.P-46**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Spectroscopic Characterization and Reactivity of a Non-Heme Cobalt(IV)-Oxo

Jindou Yang, Mi Sook Seo[1], Yong-Min Lee[2], Wonwoo Nam[*]

Department of Chemistry and Nano Science, Ewha Womans University, Korea
[1]*Institute of Nano & BioTechnology, Ewha Womans University, Korea*
[2]*Research Institute for Basic Sciences, Ewha Womans University, Korea*

High-valent metal-oxo species are of great interest as highly reactive intermediates in the catalytic oxidation of organic substrates and water by enzymes and biomimetic compounds.[1] Since these metal-oxo moieties have been fully characterized, many model complexes have further been investigated their reactivity in various oxidation reactions, such as oxygen atom transfer (OAT) and C-H bond activation reactions. Recently, the characterization and reactivity of high-valent cobalt-oxo species have also been reported.[2] We herein report the generation, spectroscopic and theoretical characterization, and reactivity of a Co(IV)-oxo complex bearing an N4-macrocyclic ligand 12-TBC, $[Co(O)(12\text{-}TBC)(O)]^{2+}$ (**1**) (12-TBC = 1,4,7,10-tetrabenzyl-1,4,7,10-tetraazacyclododecane). In particular, the rRaman spectra of **1** exhibited two isotopically sensitive features centered at 782 cm^{-1}, which shift to lower energy upon ^{18}O-incorporation with altered relative intensities (centered at 745 cm^{-1}). Furthermore, EPR, EXAFS and magnetic circular dichroism (MCD) data showed a high degree of rhombicity, indicating structural distortion of a Co–O core in the complex. With the DFT calculation of the complex being distorted from tetragonal symmetry, we conclude that the oxo wall still holds, despite the presence of a Co=O double bond. The reactivity of **1** in C-H bond activation and OAT reactions is discussed as well. Reference:[1] a) Nam, W. *Acc. Chem. Res.* **2007**, *40*, 465; b) Borovik, A. S. *Chem. Soc. Rev.* **2011**, *40*, 1870.[2] Wang, B.; Lee, Y.-M.; Tcho, W.-Y.; Tussupbayev, S.; Kim, S.-T.; Kim, Y.; Seo, M. S.; Cho, K.-B.; Dede, Y.; Keegan, B. C.; Ogura, T.; Kim, S. H.; Ohta, T.; Baik, M.-H.; Ray, K.; Shearer, J.; Nam, W. *Nat. Commun.* **2017**, *8*, 14839.

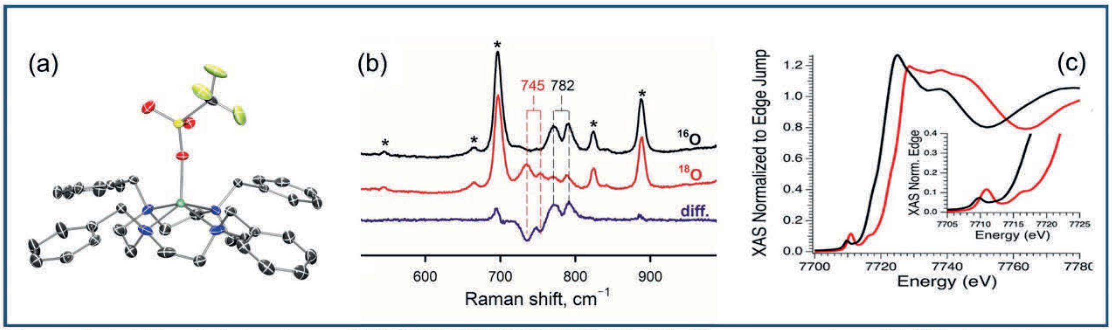


Figure 1. (a) Crystal structure of $[Co^{II}(12\text{-}TBC)(CF_3SO_3)]^+$. (b) rRaman spectra of **1**-^{16}O (black) and **1**-^{18}O (red) with λ_{ex} = 442 nm in acetone-*d*$_6$/TFE (*v*/*v* = 4/1) at –40 °C. Blue line shows the difference spectrum of **1**-^{16}O and **1**-^{18}O. (c) Co K-edge XANES of Co^{II} (black) and **1** (red).

Poster Presentation : **INOR.P-47**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Single molecule tracking of PV1 reveals ever-changing structure of diaphragmed fenestrae induced by membrane curvature mediated PV1 multimerization

Wonhee Lee, HyeongGyu Jin[1], Jiseong Park[1], Sangwon Shin[1], Yongdeok Ahn[1], Daeha Seo[1,*]

Department of New Biology, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea

To deal with loss of membrane integrity by curvature, cells are equipped with repair system mediated by membrane curvature sensing proteins, including plasmalemmal vesicle associated protein 1 (PV1). It has been proposed that entanglement of PV1 forms the diaphragm to prevent expansion of fenestrae, however, biophysical principle of diaphragmed fenestrae formation is not addressed yet. Based on single PV1 trajectories in live cell, dynamic transition between fast, slow, and immobile states of PV1 which are corresponding to dimer, dimer-of-dimer, and oligomer complex is identified. In addition, such equilibrium is shifted toward to immobile states when membrane rupture is induced. These results indicate that immobile diaphragm composed by multiple PV1 is ever-changing structure and the unstable membrane induces this structure to prevent membrane deformation. Using agent-based dynamic simulation, we proposed that density dependent diffusivity with two interaction scales is needed to generate clustering pattern. This result gives us a unique insight into fenestrae formation in terms of the collective behavior of PV1.

Poster Presentation : **INOR.P-48**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Interrelationships between Vitamins and Matrix Metalloproteinase-2

Sumin Park, Hyuck Jin Lee[*]

Department of Chemistry Education, Kongju National University, Korea

Matrix metalloproteinases (MMPs) are known as many pathological indicators, including Alzheimer's diseases (AD). Particularly, high levels of MMP-2 has been observed in AD patients' brain. Moreover, MMP-2 could directly degrade amyloid precursor protein (APP) and amyloid-β (Aβ), which are considered as the main risk factors of AD. On this account, MMP-2 has been suggested to be related to the occurrence and progression of AD. In this study, we investigated the effect of both fat- and water-soluble vitamins [i.e., retinol (vitamin A), pyridoxamine (vitamin B6), ascorbic acid (vitamin C), and cholecalciferol (vitamin D3)] on activity of MMP-2. The interactions between vitamins and MMP-2 were identified through docking simulations and the enzymatic activity of MMP-2 in the presence of vitamins was determined through zymography. As a result, vitamins could inhibit the activity of MMP-2 by interacting with the enzyme near the active site. By investigating the relationships between biomolecules, such as vitamins, and MMP-2 can help understanding the influence of MMP-2 on the etiology of AD.

Poster Presentation : **INOR.P-49**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Steric Control of Linear Carbene-Au(I)-Amide Complexes for High-Efficiency Electroluminescence

Seunga Heo, Kyungmin Kim[1], Yongsik Jung[2], Joonghyuk Kim[3], Hye Jin Bae[3], Hyeonho Choi[4], Jaeheung Cho[5,*], Youngmin You[*]

Chemical Engineering and Materials Science, Ewha Womans University, Korea
[1]*Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*
[2]*Samsung Advanced Institute of Technology (SAIT), Samsung Advanced Institute of Technology, Korea*
[3]*Samsung Advanced Institute of Technology, Korea*
[4]*Material Research Center, Samsung Advanced Institute of Technology, Korea*
[5]*Department of Chemistry, UNIST, Korea*

Linear carbene-Au(I)-amide complexes have emerged as promising materials for high-efficiency organic light-emitting devices (OLEDs). However, the Au(I) complexes suffer from rapid non-radiative deactivation due to excited-state geometric changes. To circumvent this limitation, we designed a series of Au(I) complexes having sterically hindering ligands, including the 1,3-bis(2,6-diisopropylphenyl)-1H-benzo[d]imidazol-2-ylidene ($^{\text{Dipp}}$BZI) carbene and the 1,3,6,8-tetramethyl-9H-carbazolide (TMCz) amido ligands. This molecular design was anticipated to minimize excited-state reorganizations including the dihedral distortion and the Renner-Teller distortion. 1,3-Diphenyl-1H-benzo[d]imidazole-3-ylidene (BZI) and carbazolide (Cz) served as controls to prepare four complexes, [Au($^{\text{Dipp}}$BZI)(TMCz)], [Au($^{\text{Dipp}}$BZI)(Cz)], [Au(BZI)(TMCz)], and [Au(BZI)(Cz)]. X-ray single crystal analyses revealed pseudo-linear geometries with different bent and dihedral angles. All the complexes exhibited strong photoluminescence emission in Ar-saturated toluene. [Au($^{\text{Dipp}}$BZI)(TMCz)] with the largest steric volume exhibited the largest photoluminescence quantum yield of 0.79. An external quantum efficiency as high as 16.5% was recorded for the device of ITO (10 nm)/NDP-9 (10 nm)/HT211 (40 nm)/oCBP(10 nm)/HT host:ET host:10% [Au($^{\text{Dipp}}$BZI)(TMCz)] (30 nm)/mCP-2CN (10 nm)/DPFPO:LiQ (15 nm)/LiQ (1 nm)/Al (100 nm). Our study demonstrates the effectiveness of the steric control toward improved luminescence efficiencies.

Poster Presentation : **INOR.P-50**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Rotational dynamics of endocytic vesicle during intracellular transport

HyeongGyu Jin, Daeha Seo*

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

Intracellular cargos, such as organism, protein, and endocytic vesicles, are transported by the molecular motor proteins along cytoskeletal network. The mechanical competition of kinesin and dynein, called a ‘‘tug-of-war,’’ leads to bidirectional transport of cargo which is involved in cellular function, development, and disease. However, how their dynamics lead to frequent pause or switch in intersection of microtubule is unclear due to technical challenge for observing attachment or detachment of motor protein in living cell. Here, we present long-lasting dark-field microscopy to observe position and orientation of endocytic vesicle using gold nanorod. We demonstrate accuracy of spatial and angular information in numerical experiments. And we reveal which axis, how often, and how much rotation occurs at pause. This method offers a strategy to observe 3D rotational motion in real time, and provides unique insights into the mechanism underlying the molecular dynamics for motor proteins.

Poster Presentation : **INOR.P-51**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Optical microscopic revelation of hot-electron effect in plasmonic photocatalysts

Yongdeok Ahn, Daeha Seo*

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

Plasmonic metals have been spotlighted as a photo-catalytic materials due to their large absorption to visible-light. Although their photocatalytic activity is insufficient comparing to semiconductors, plasmonic metals contribute to enhance the ability of heterogeneous catalysts under irradiation through transferring energy and electrons. Especially, interband excitation (5d to 6sp) in Au showed the potential to generate charge separation effectively much as conventional photocatalysts in several studies. Here, we focused on the different thermodynamics of hot electrons depending on generating pathway and expected that they show different contribution as photosensitizer. Additionally, to understand photocatalytic contribution of charge transfer excepting other rate determining steps at single particle level on optical microscope, we developed observing method. This method provides uniform initial condition for each nanocatalyst to avoid stability problem not only selective kinetic information. We, successfully, distinguished the effective contributions of two different excitations in plasmonic metals. We also revealed another mechanism of hot electron transfer from plasmonic metal to semiconductor at single particle level.

Poster Presentation : **INOR.P-52**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Detection of Membrane Phase Separation by Long Term Single Molecule Observation

Jiseong Park, Daeha Seo*

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

In live cell, plasma membrane is in dynamic equilibrium between the different phases. The interaction of molecules with the ordered phase, i.e., lipid raft, influences their trafficking as well as downstream signal regulation. Here, we tracked single lipid molecules with high localization accuracy (

Poster Presentation : **INOR.P-53**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Effect of Cation and Transition Metal for Determining Crytal Structure andElectronic Properties on the Zintl phase $Ba_{1-x}Sr_xZn_{2-y}Cd_ySb_2$ System

Jiwon Jeong, **Tae-Soo You**[1,*]

Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Thermoelectric (TE) materials and the devices based on these materials have been considered as one of the smartest approaches to reduce global energy consumption by recovering the waste heat from various heat sources and converting it into electricity. Zintl phase can be considered as one type of intermetallic compound composed of electropositive alkali and alkaline-earth metals elements and electronegative main-group metals or semimetal. Recently, the $A M_2 Pn_2$ (A = Mg, Ca, Sr, Ba; M = Mn, Zn, Cd; Pn = P, As, Sb, Bi) series has been extensively investigated as Zintl phase TE materials, and three major structure types have been identified: the $ThCr_2Si_2$-type having metallic behavior, the $CaAl_2Si_2$-type and the $BaCu_2S_2$-type both showing the semiconducting behavior. Interestingly, the compounds in the BaM_2Sb_2 (M = Mn, Zn, Cd) system adopted several different structure types depending on the used transition metals. For instance, $BaMn_2Sb_2$, $BaZn_2Sb_2$, and $BaCd_2Sb_2$ adopt the $ThCr_2Si_2$-type, the $BaCu_2S_2$-type, and the $CaAl_2Si_2$-type, respectively. To investigate the effect of these transition metals for the refined structure types having semiconducting behavior, the solid-solution quaternary Zintle phase $BaZn_{2-x}CdxSb_2$ system containing the Zn/Cd mixed-site was synthesized by a conventional high-temperature synthetic method and Pb-flux method to increase crystallinity. Besides, to understand the effect of cation for determining the crystal structure, we mixed $SrZn_2Sb_2$ adopting $CaAl_2Si_2$-type with $BaZn_2Sb_2$ adopting $BaCu_2S_2$-type respectively. Their crystal structures were characterized by both powder and single-crystal X-ray diffractions. From the X-ray diffractions, it is found that not only the structural volume increases as the amount of Cd increases but also a single phase was formed when transition metal was introduced below 25% and cation was introduced below 20%. Interestingly, the structure selectivity from mixed-phase to single-phase was increased when crystallinity was improved by the Pb-flux method. A series of theoretical calculations using three hypothetical models was performed by the tight-binding linear muffin-tin orbital (TB-LMTO) method,

and the resultant DOS and COHP curve analyses were thoroughly studied resulting in the band-gap opening occur when cation mixing and transition metal mixing were done.

Poster Presentation : **INOR.P-54**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Experimental and Theoretical Studies for the Zintl Thermoelectric $Ca_{3-x}Yb_xAlSb_3$ System

Yeongjin Hong, **Tae-Soo You**[1,*]

Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Thermoelectric (TE) materials and devices have great potential in reducing energy crises and losses by converting wasted heat into useful energy. Zintl phase can be considered as an intermetallic compound composed of electropositive alkali and alkaline-earth metals elements and electronegative main-group metals or semimetal. Zintl phase compounds are valuable for thermoelectric applications at high temperatures. Several examples of these Zintl thermoelectric materials are as follows: $A_{14}MSb_{11}$ (A = Ca, Yb; M = Mn, Al), $A_5Al_2Sb_6$ (A= Ca, Yb), $A_{11}Pn_{10}$ (A = Ca, Yb; Pn = Sb, Bi, Sn), A_2CdSb_2 (A = Ca, Yb, Eu), and A_3MSb_3(A = Ca, Sr; M = Al, Ga) series. Among the Zintl phase thermoelectric compounds, the A_3MPn_3 (A = Ca, Sr, Ba, Eu ; M = Al, Ga, In; Pn = Sb, As, P) system has been reported to have five different structure types, such as orthorhombic Ca_3AlAs_3(*Pnma*), Ba_3AlSb_3(*Cmce*), Ba_3GaSb_3(*Pnma*) and monoclinic Sr_3GaSb_3($P2_1/c$), Rb_3TiO_3($P2_1/c$). In particular, Ca_3AlSb_3 was known to have the Ca_3AlAs_3 structure type and composed of infinite chains of corner-sharing $AlSb_4$ tetrahedra. The novel Zintl phase series $Ca_{3-x}Yb_xAlSb_3$ ($0≤x≤0.82(2)$) is consist of three compound as Ca_3AlSb_3 (loaded composition $Ca_3AlSb_{2.7}Ge_{0.3}$), $Ca_{2.59(2)}Yb_{0.41}AlSb_3$, $Ca_{2.18(2)}Yb_{0.82}AlSb_3$. These compounds were synthesized by the arc-melting method and Pb metal-flux reaction, and bar shaped crystal growth was performed through the metal flux reaction. Also their crystal structures were characterized by both powder and single-crystal X-ray diffractions. Dopants including Yb, Ge in the $Ca_{3-x}Yb_xAlSb_3$ system is Ca-rich compound. Quite interestingly, $Ca_{3-x}Yb_xAlSb_3$ initially crystallized in the mixed-phase, but after post-heat treatment, those were converted to the orthorhombic Pnma space group (Z = 4, Pearson Code *oP*28) and successfully transformed to the Ca_3AlSb_3 crystal structure. However, the p-type dopant of Ge was not included. To understand the electronic structure of the title compounds, a series of theoretical calculations using the TB-LMTO method was performed, and the resultant DOS and COHP analyses were thoroughly conducted. In particular, as Ca and Yb are mixed, the DOS level was relatively lower at the Fermi level, and this region was slightly wider than the other compounds. The chemical composition analyzed by EDS indicated $Ca_{2.59(2)}Yb_{0.41}AlSb_3$, which was quite close to the SXRD result. The thermal stability of $Ca_{2.59(2)}Yb_{0.41}AlSb_3$ was investigated by TGA. Also as a result of the physical property measurement, it is confirmed that the electrical conductivity increases up to 500K, indicating that it exhibits semiconductor properties.

Poster Presentation : **INOR.P-55**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Effect of cations on substitution of double-one divalence Rare-Earth-Metal for the Zintl Thermoelectric $Ca_{5-x-y}Yb_xEu_yAl_2Sb_6$ ($0 \leq x \leq 1.12(2)$; $0 \leq y \leq 0.63(2)$) System

Yeongjin Hong, **Tae-Soo You**[1,*]

Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Thermoelectric (TE) materials and devices have great potential in reducing energy crises and losses by converting wasted heat into useful energy. The $A_5M_2Pn_6$ (A = Ca, Sr, Eu, Yb; M = Al, Ga, In) series has been extensively investigated as Zintl phase TE materials, and two major structure types have been identified: the $Ca_5Al_2Bi_6$-type having metallic behavior and the $Ca_5Ga_2As_6$-type showing the semiconducting behavior. To investigate the effect of cationic substitution and double substitution for TE properties of the $Ca_5Ga_2Sb_6$-type compounds, quarternary and quinary Zintl phase $Ca_{3.57(2)}Yb_{1.12}Eu_{0.31(1)}Al_2Sb_6$, $Ca_{4.37(2)}Eu_{0.63}Al_2Sb_6$ was successfully synthesized by arc-melting and Pb-metal flux method. Bar-shaped crystal growth was performed through the metal flux reaction. Also, their crystal structures were characterized by both powder and single-crystal X-ray diffractions. The novel Zintl phase belonging to the $Ca_{5-x-y}Yb_xEu_yAl_2Sb_6$ system was a Ca-rich compound, adopts the $Ca_5Ga_2As_6$-type structure, those were converted to the orthorhombic *Pbam* space group (Z = 2, Pearson Code *oP*26). To understand the electronic structure of the title compounds, a series of theoretical calculations using the TB-LMTO method was performed, and the resultant DOS and COHP analyses were thoroughly conducted. The chemical composition analyzed by EDS indicated $Ca_{2.57(2)}Yb_{1.12}Eu_{0.31(1)}Al_2Sb_6$, which was quite close to the SXRD result. Also, Magnetic property measurement for $Ca_{4.37(2)}Eu_{0.63}Al_2Sb_6$, confirmed the antiferromagnetic (AFM) interactions of Eu elements at relatively low-temperature paramagnetic Curie temperatures of -29.08K.

Poster Presentation : **INOR.P-56**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Characterization of Single Atomic Rh Decoration of Pt Nanocubes and Application towards the Direct Ethanol Fuel Cells

MiJi KiM, Hye Jin Lee, Jeonghyeon Kim, Sang-Il Choi*

Department of Chemistry, Kyungpook National University, Korea

- Withdrawal -

Poster Presentation : **INOR.P-57**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Co catalysts derived from Zeolitic-imidazolate Framework-8 (ZIF-8) and their catalytic performances for the air electrodes in Zn-air batteries

Gyungse Park*, <u>Sheraz Ahmed</u>[1]

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

Co/ZIF-8 catalysts were obtained by the calcination of ZIF-8. A general and high-yield strategy for the formation of Co/ZIF-8 catalysts from the zeolitic-imidazazolate framework (ZIF-8) developed at a temperature of 1050 ˚C by the calcination process. The purpose for the formation of Co doped on carbon derived from ZIF-8 is to obtain small nanocatalysts with high activity. The formation of Co and their oxides was investigated by the X-ray diffraction (XRD) and the graphitization was analyzed by the Raman Spectroscopy. The resulting Co/ZIF-8 are highly porous with a high specific surface area of 329.4 m^2/g. Furthermore, the porous Co/ZIF-8 exhibited superior electrochemical performance when applied as a cathode material for the Zn-air batteries. The cyclic test for charging and discharging was performed for 500 h revealing a potential catalyst, having splendid stability for the OER and ORR in the Zn-air batteries. The excellent electrochemical performance for these catalysts may be attributed to the various factors. Including (i) presence of porous carbon prevents from aggregation (ii) the high porosity increases the active sites (iii) the calcination under nitrogenous atmosphere improves the conductivity for the frameworks.

Poster Presentation : **INOR.P-58**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Tip-to-Middle Anisotropic MOF-on-MOF Growth with a Structural Adjustment

Gihyun Lee, Sujeong Lee, Sojin Oh, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The construction of well-organized hybrid metal-organic frameworks (MOFs) with complicated structures or components is a great importance because of their potential usefulness. In this regard, the conjugation of more than two MOFs, which have dissimilar components and/or structures, is a smart strategy for the production of hybrid MOFs. Herein, we report an interesting MOF growth process for the construction of hybrid MOF containing heterogeneous components and cell lattices. Interestingly, even though a newly grown MOF and a MOF template have mismatched cell lattices, the anisotropic growth results in unexpectedly well-defined core–shell-type hybrid MOFs. Comprehensive monitoring of the growth process revealed a tip-to-middle MOF-on-MOF growth, which elucidates the uncommon formation of a well-defined core–shell hybrid despite the anisotropic growth. A tip-to-middle anisotropic growth process is accompanied with self-adjustment of MOF cell lattices to anchor on the template surface having mismatched cell lattices in the early reaction stage, and self-reversion of cell lattices to the original comfortable configuration in the middle stage of the reaction.

Poster Presentation : **INOR.P-59**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

ZIF Composite Incorporated with CoNi Nanoparticles for Efficient Catalytic Reaction

Sojin Oh, Sujeong Lee, Moonhyun Oh*

Department of Chemistry, Yonsei University, Korea

The incorporation of metal nanocatalysts within a well-defined porous support is of great importance to stabilize unstable metal nanocatalysts for the effective and long-lasting catalytic reaction. Within this aspect, metal-organic frameworks (MOFs) are the excellent supports to stabilize unstable nanocatalysts. Moreover, the development of non-expensive metal nanocatalysts is important to replace expensive novel metal nanocatalysts. Herein, we report a simple method for the preparation of a porous ZIF-based and a carbon-based composites incorporated with catalytic active CoNi alloy nanoparticles. CoNi alloy nanoparticles are produced from the concurrent reduction of cobalt and nickel ions existing within the ZIF-based precursor material during the thermal treatment. The synergetic effect between a highly porous ZIF support and well-dispersed CoNi nanoparticles within CoNi@ZIF-400 provides an outstanding catalytic performance even though the incorporation of non-expensive nanoparticles.

Poster Presentation : **INOR.P-60**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Preparation of Metal-Organic Framework Papers and Their Selective Dye Separation

<u>Haejin Kwon</u>, Moonhyun Oh[*]

Department of Chemistry, Yonsei University, Korea

The conjugation of metal-organic frameworks (MOFs) with other materials is an excellent approach for the development of innovative MOF materials with superior properties and/or wider applicability. In particular, the conjugation of MOFs (specially, water stable MOFs) with a flexible filter paper would provide a rapid, facile, and convenient route for the generation of flexible MOF materials that could be useful for the separation of pollutants in water. Herein, we report the conjugation of MOF and filter paper for the production of MOF papers. The flexible CMFP/MOF materials possess a compact and uniform growth of MOF nanoparticles on the cellulose surface of the carboxymethylated filter paper (CMFP). An effective and simple separation of organic dyes from an aqueous solution was demonstrated by using the prepared CMFP/MOF.

Poster Presentation : **INOR.P-61**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Enhancement of Catalytic Activity of MOF by Providing Structural Defects

Hyeji Jun, Sojin Oh, Gihyun Lee, Moonhyun Oh[*]

Department of Chemistry, Yonsei University, Korea

The well-developed micropores of metal-organic frameworks (MOFs) are highly advantageous for convenient mass transfer during the catalytic reactions, and the open metal sites within MOFs are the active sites in a catalytic application. However, most of the metal sites in MOFs are already coordinated to organic linkers as a part of their framework, and hence, it is hard for the reactants to access the active metals. Therefore, the construction of crystalline MOFs having numerous open metal sites is an ultimate strategy for the construction of highly active MOF catalysts. Herein, we report a strategy for the enhancement of catalytic activity of MOF by providing the intentional structural defects within a MOF structure.

Poster Presentation : **INOR.P-62**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Solid-state conversion of tetrathiafulvalene crystals for highly conductive mixed-valence crystals

Yoolim Ahn, Hee Cheul Choi[*]

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

Solid-state conversion by a spontaneous redox reaction between tetrathiafulvalene (TTF) and ferric ion is employed to obtain morphology-retained TTF mixed-valence (MV) crystals. There are considerable interests in organic MV crystals for both fundamental studies and their applications as electronic device components. A challenge facing their efficient device application is to obtain the final MV crystals in device-friendly shapes. However, it is quite difficult because the conventional method to obtain organic MV crystals requires two steps: (1) generation of radical molecules, followed by (2) crystallization of the radical species together with neutral species, which does not guarantee the shape of the final product. A potential solution for this would be to develop a new method that converts neutral crystals in a specific shape to MV crystals without destroying the original shape. This issue can be resolved by employing a simple spontaneous redox reaction to generate radicals directly in pre-made organic molecular crystals. We demonstrate this with the redox reaction between TTF crystals and ferric ion solution and revealed the underlying mechanism by time-dependent observations. The electrical conductivity of the resulting crystals increased by six orders of magnitude. It also shows the potential of conductivity modulation by controlling the oxidant concentration. By taking the advantage of solid-state conversion, TTF neutral-MV hetero-structures were demonstrated by selectively contacting TTF crystals to ferric ion solution, and they were applied to self-contact devices, which showed higher conductance values than the silver paste devices. We believe that this achievement will contribute to developing MV radical crystals and their applications in electronic devices.

Poster Presentation : **INOR.P-63**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Viscosity-dependent Concave and Branched Morphologies of Fullerene C_{70} Molecular Crystals

Kwangjin Song, Hee Cheul Choi[*]

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

In this presentation, we report that a kinetic overgrowth allowing organic molecular crystals in various morphologies is induced by temperature-dependent viscosity change of crystallization solution. Over the decades, strategic control of the morphology of metal nanocrystals have been studied widely because different exposed facets of each morphology show extremely different optical, electrical, and catalytic properties. However, such study is limited for organic molecular crystals because of their intrinsic anisotropy. Herein, we revealed that temperature decrease during antisolvent crystallization (ASC) induces viscosity increase of crystallization solution, so slow down the diffusion rate of solute, which promotes the kinetic overgrowth at edges and vertices of cubic fullerene C_{70} crystals. Structural analysis using powder X-ray diffraction (PXRD) and time-dependent scanning electron microscopy (SEM) studies clearly show the diffusion-rate dependent morphological changes. In addition, the importance of viscosity change on morphology control is revealed by control experiment by using acetone as antisolvent. This strategic method will promote the morphology controls of various organic molecular crystals, and boost the morphology–property relationship study of them.

Poster Presentation : **INOR.P-64**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Formation of Highly Pure Pentacene Crystals through Efficient Suppression of Dihydropentacene Impurity during Physical Vapor Transport Process

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*

Pentacene, the franchise star of organic semiconductors, has been suffering from unavoidable impurities represented by dihydropentacene (DHP). Although they should be eliminated for the development of high-performance devices and the fundamental research, no efficient way to avoid DHP is available yet. Here, we present that highly pure pentacene crystals are obtained in high yield by using physical vapor transport process with H_2 carrier gas. While other popular carrier gases including Ar and N_2 result in dihydropentacene-pentacene cocrystals as a major product, only H_2 carrier gas results in pure pentacene crystals. This happens by effectively suppressing the disproportionation reaction of pentacene, which largely owes to its reaction with DHP. The efficient formation of highly pure pentacene crystals directly from commercial raw precursors will contribute to the systematic studies on pentacene as well as developments of novel strategies for the growth of high purity organic semiconducting materials.

Poster Presentation : **INOR.P-65**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Highly efficient TADF emitters based on boron-carbonyl hybrid acceptors with fast spin-flip process

Ina Nur Istiqomah, Young Hoon Lee, Hanif Mubarok, JuHyeong Kim, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

We report two highly efficient green and orange TADF emitters (TMCzBCO and DMACBCO) comprised of 1,3,6,8-tetramethyl-9*H*-carbazole (TMCz) or 9,9-dimethyl-9,10-dihydroacridine (DMAC) donors and planar boron-carbonyl (BCO) hybrid acceptors. Both emitters exhibited high photoluminescence quantum yields (Φ_{PL}= ~94%), a small singlet-triplet energy gab (ΔE_{ST} = ~0.01 eV), and very short delayed fluorescence lifetime (~1 μs). These results indicate that a $^3n\pi^*$ state of the BCO unit acting as an intermediate local triplet excited state (^{3}LE, T_2) leads to improving RISC rate (k_{RISC} = >10^6 s^{-1}) and shortening the excition lifetime due to the large spin-orbit coupling between the T_2 and excited singlet (S_1) states with low activation energy less than 10 meV. As a result, the TADF-OLEDs devices also show high performance with EQE of 24.7% for the green TMCzBCO and 28.4% for the yellow DMACBCO emitters, respectively. Remarkably, the devices maintain high efficiency at high lumiance exceeding 20% at 5,000 cd m^{-2} and 18% at 10,000 cd m^{-2}.

Poster Presentation : **INOR.P-66**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and TADF properties of boron emitters comprising rigid donor and acceptor units linked by a carbon-carbon bond

Ki Hoon Shin, Nhi Nguyen Ngoc Tuyet, Jin Seon Cha, Min Hyung Lee[*]

Department of Chemistry, University of Ulsan, Korea

We report three rigid donor (D)-acceptor (A)-type thermally activated delayed fluorescence (TADF) compounds, CzMeBCO (**1**), BuCzMeBCO (**2**), and EtCzMeBCO (**3**), in which 9-substituted 9*H*-carbazole (9-RCz) donors are linked with a boron-carbonyl (BCO) hybrid acceptor by a carbon-carbon bond. In toluene solution, all compounds exhibit normal fluorescence in deep blue region (426-429 nm) with high photoluminescence quantum yields (PLQYs) of 77%-93% whereas they exhibit greenish blue to green emissions in PMMA film with distinct delayed fluorescence components. High PLQYs are also retained in their rigid state, showing 60%-85% in PMMA film. However, the PLQY and delayed fluorescence lifetime decrease with the increase of the doping concentration of compounds in the film state. The details of synthesis and photophysical properties of compounds will be discussed with theoretical study.

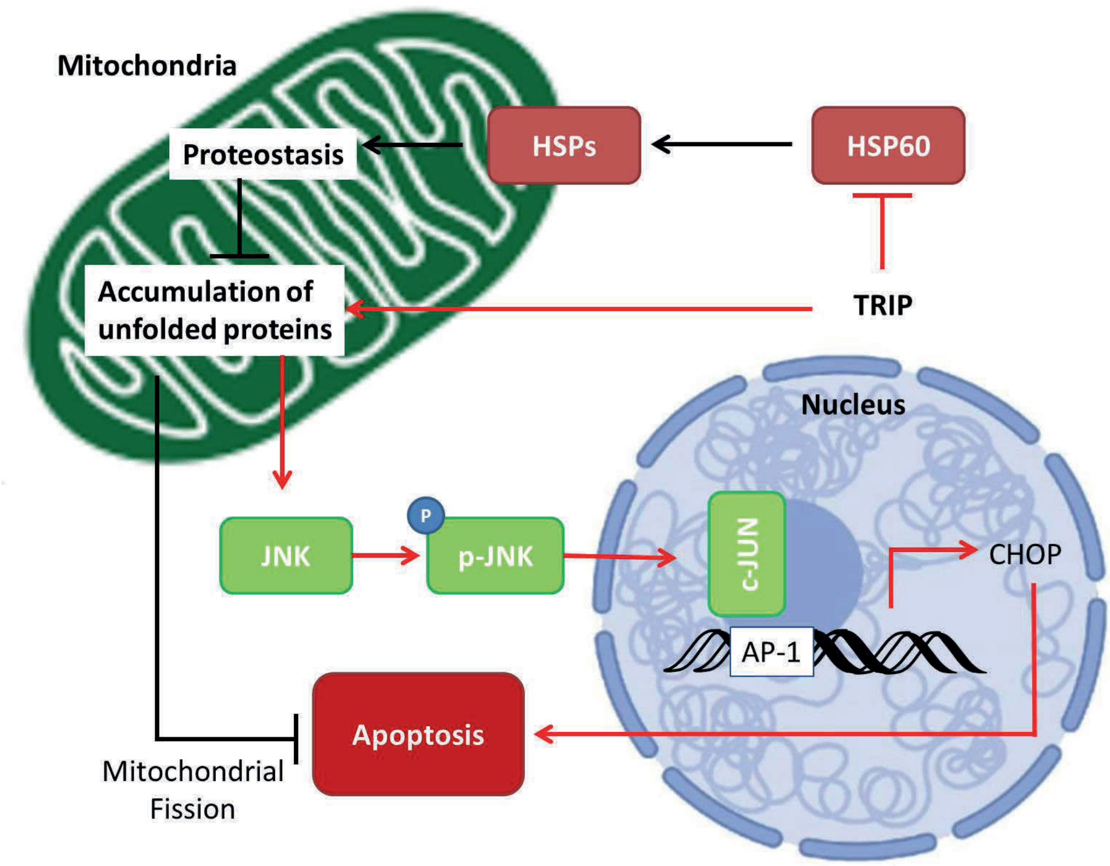
Poster Presentation : **INOR.P-67**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A rhenium isonitrile complex induces HSP60-mediated mitochondrial apoptosis.

Junhyeong Yim, Seung Bum Park[1,*]

BioPhysics and Chemical Biology, Seoul National University, Korea
[1]*Division of Chemistry, Seoul National University, Korea*

Many inorganic compounds, like Platin derivatives, are used to treat cancer. Interestingly, Rhenium-based compounds also showed anti-cancer effects. But unlike Platinum-based compounds like Cisplatin or Carboplatin, which are DNA crosslinkers, the mechanism that how Rhenium-based compounds showed anti-cancer effects is still unclear. So We are going to reveal and validate the target protein of Rhenium Isonitrile Complex (TRIP), and to clarify the Mechanism of Action (MoA) of TRIP against cancer cells via our novel target ID method, label-Free Target Identification Using In-Gel Fluorescence Difference via Thermal Stability Shift, called TS-FITGE. TS-FITGE revealed the target protein of TRIP as HSP60, which works as a chaperonin. Inhibit HSP60 by TRIP induces accumulation of misfolded proteins at mitochondria. Misfolded proteins activate CHOP via JNK2/p-JNK2 pathway. CHOP activation may induce mitochondrial apoptosis of cancer cells.


Mitochondria
Proteostasis
HSPs
HSP60
TRIP
Accumulation of unfolded proteins
Nucleus
P
JNK
p-JNK
c-JUN
CHOP
AP-1
Apoptosis
Mitochondrial Fission

Poster Presentation : **INOR.P-68**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Sunlight Activatable ROS Generator for Cell Death Using TiO_2/*c*-Si Microwires

Sangwon Shin, Wonhee Lee[1], Daeha Seo*

Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Dept. of New Biology, Daegu Gyeongbuk Institute of Science & Technology, Korea*

For cell death and water purification, photocatalytic reactive oxygen species (ROS) generation is an engaging and efficient technique due to time and location specific manner. However, it is challenging to analyze the generated ROS quantitatively and qualitatively because of the reactive chemical properties and short lifetime. Here, we use new ROS generation system consisting of tapered crystalline silicon microwires coated with anatase titanium dioxide for a conformal junction, resulting in effective ROS generation. By analyzing the cellular damage and cell cytotoxicity, we predict the generated ROS species and quantity indirectly. Comparing the cell cytotoxicity with H_2O_2, we revealed that only 15 min light irradiation on the system was comparable to the conventional germicidal level of H_2O_2 (~ 3mM). Logical regression analysis with cellular survival data revealed that the diffusion length of the ROS is ~ 9 μm, inferring that the most dominant species causing cell damage is H_2O_2.

Poster Presentation : **INOR.P-69**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Water Induced Structural Change and Proton Motion Study in Crystalline Porous Materials

Younghu Son, Jiyun Kim, Minyoung Yoon[1,*]

Department of Chemistry, Kyungpook National University, Korea

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

Electric energy is working with the movement of electrons, a negatively charged particle in an energy system. For the compensation of the charge, positively charged particles such as an ion must move to the opposite direction of electrons. Among the various positively charged ions, a proton, the smallest cation, is commonly involved in biological and chemical electric energy systems. The proton pump or proton channels are common proton transport systems in biological energy systems. However, the detailed study of proton motion and mechanism has been scarcely done in chemical proton transport systems. For the study of proton conduction mechanisms in chemical systems, structural elucidation of the system is one of the most critical issues and therefore metal-organic frameworks (MOFs) provide a unique platform due to their designability, crystallinity, and porosity. In this study, we employed various microporous metal formates, $M(HCO_2)_2$, where M = Mg(II), Co(II), Ni(II), for the study of proton conduction behavior and mechanism. The structure of MOFs was analyzed by single-crystal structure analysis, which was further confirmed by powder X-ray diffraction (PXRD) analysis. Interestingly, the structure of MOFs was changed upon exposure to humidity and proton conductivity and water vapor adsorption follow similar trends to the structure change. The details of the framework structure and the related proton conductivity depending on the relative humidity were analyzed. For the detailed understanding of proton motion in the crystal structure, ^{2}H NMR was used to propose a proton conduction mechanism in the MOFs. In addition, for the detailed analysis of proton position and dynamics, neutron diffraction and scattering techniques were also employed. The details of this work will be presented.

Poster Presentation : **INOR.P-70**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Supramolecular Polymerization Based on Porphyrin Metalation in Aqueous Media

Sukyoung Kim, Sung Ho Jung[1,*], Jong Hwa Jung[*]

Department of Chemistry, Gyeongsang National University, Korea
[1]*Liberal Arts/Chemistry, Gyeongsang National University, Korea*

Self-assembly is a powerful strategy to access functional supramolecular nanostructures from small molecules, which show great promise for applications ranging from advanced materials and organic electronics to biomedical engineering. Herein, we report the metalation-dependent assembling behavior shown by porphyrin derivative, which formed different supramolecular polymers with/without Zinc ions in aqueous media, that is, H-aggregation (nanoparticles) and J-aggregation (nanosheet with Zn), respectively. Supramolecular polymers were characterized by UV-Vis spectrometry and atom force microscopes (AFM). We have studied the growth kinetics of these supramolecular polymers, the self-assembled metalloporphyrin via Zinc (II) ions insertion into free-base porphyrin in equilibrated H-type aggregates. We present that the nanosheets area was controlled by adding varying amounts of nanoparticles in their kinetically trapped state with Zinc ions to the seed nanosheet. These results will contribute to the design of supramolecular systems.

Poster Presentation : **INOR.P-71**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Preparation of heterogeneous aryl-Pd(II)-oxo clusters via surface oxidation for C-H arylation

Minjun Kim, Hyunwoo Kim[*], Hyunjoon Song[*]

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

Arylated hetero-aromatic compounds are valuable structural motifs present in many natural molecules and bioactive compounds. Most C-H arylation of hetero-aromatic compounds have been proceeded via homogeneous transition metal-catalyzed C-C coupling reactions. However, homogeneous catalysts have drawbacks that they are difficult to separate and reuse. Recently, Glorius and co-workers used heterogeneous Pd/C catalyst for C-H arylation of hetero-aromatic compounds using diaryliodonium oxidants and confirmed high reactivity and selectivity to thiophene, benzo[b]thiophene, and other hetero-aromatic compounds. However, the structure of Pd/C used was not well-defined, so it was difficult to analyse the active species, then the reaction mechanism was inferred through kinetic analysis.In this study, we characterized the active species for C-H arylation of hetero-aromatic compounds via diaryliodonium oxidant and identified the reaction mechanism. Well-defined Pd NPs with average size of 3.5 nm were used to analyse the exact structure and mechanism. Preferentially, we confirmed that C-H arylation of indole and benzofuran using Pd NPs and oxidant had high yield and selectivity at C2-position. X-ray photoelectron spectroscopy (XPS) and X-ray absorption fine structure (XAFS) were used to confirm the active species from interaction of Pd NPs and oxidants. We identified that the intermediate is composed of Pd(II) species stabilized by oxo- and aryl group.

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Poster Presentation : **INOR.P-72**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Selective Photocatalytic Production of Benzyl Alcohol to Benzaldehyde or Deoxybenzoin by Ion exchanged CdS

SungGyu Lee, Hyun Sung Kim[1,*], Yerim Son[2]

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

In catalyst development, it is a very fundamental issues to establish the strategy for optimizing the conversion efficiency and increasing the selectivity of the valued added product. In this study, the visible light absorbing CdS nanoparticles partially were modified $Au_2$2S and Ag_2S via simple cation exchange to be heterostructure photocatalyst (denoted as Au_2S@CdS and Ag_2S@CdS) and were employed as photocatalyst for conversion of aromatic alcohol to valued added products such as benzaldehyde and C-C coupling product including deozybenzoin and hydroxybenzoin. When Au_2S@CdS is used as a photocatalyst, the main product is benzaldehyde with 99% selectivity, and when Ag_2S@CdS is used as a photocatalyst, the main product is deozybenzoin and hydroxybenzoin with 95% selectivity. The critical photogenerated electron and hole transfer during photocatalytic reaction were systemically investigated with various control experiments and in-situ high resolution X-ray photoelectron spectroscopy.

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Poster Presentation : **INOR.P-73**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Catalytic Reduction of Nitroarenes by Using Microporous Copper Silicate Spported Copper Nanoparticles

Seojin An, Yealin Tak, Yu Jin Jung, Yeojeong Jo, Hyun Sung Kim[1,*]

Chemistry , Pukyong National University, Korea
[1]Chemistry, Pukyong National University, Korea

In the copper nanoparticle catalytic system, numerous factors such as the size, morphology, exposed facet, chemical composition and so on should be seriously considered to improve catalytic performance to reach homogeneous catalytic system. Among them, the dispersity is one of the key factors for the enhancement of catalytic properties. For improve the dispersity, porous media were employed for supporting copper nanoparticles. Herein, we have demonstrated, for the first time, that copper nanoparticles can effectively be generated through reduction of Cu(II) to Cu(0) in [CuO4]2- of the SGU-29 framework using hydrogen gas. This method offers some of advantages, such as convenient synthesis of metallic Cu NPs, it does not require higher temperatures, longer reaction times, additional base, or solvent. Furthermore, reduced SGU-29 exhibited high catalytic performance for the reduction of nitroarenes with providing 99% conversion after consecutive five times without any significant drop in catalytic activity.

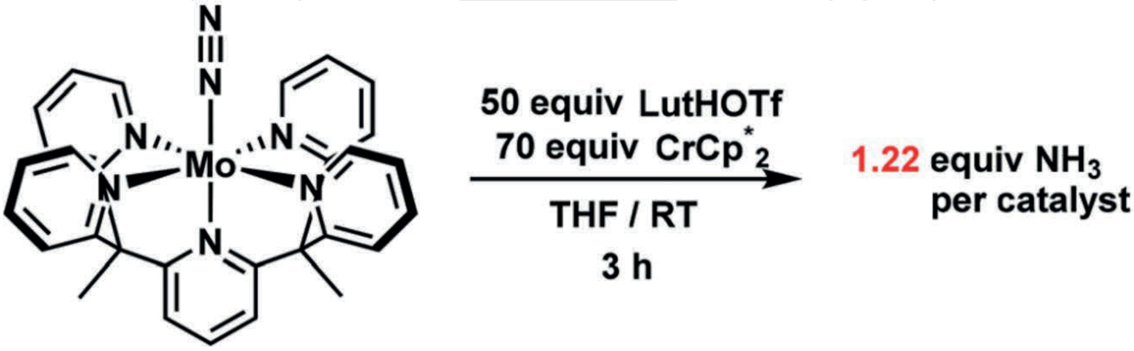
Poster Presentation : **INOR.P-74**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Dinitrogen Activation by Penta-pyridyl Molybdenum Complex

<u>Jeongmin Cha</u>, Eunsung Lee*, Hayoung Song

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

A new dinitrogen (N2) molybdenum(0) complex supported by penta-pyridine ligand was synthesized. The activated nature of the N2 ligand was elucidated by the X-ray crystal structure of the complex, which was consistent with a low N–N IR stretching frequency. The strong π-backdonation arising from the large p orbital character in molybdenum lone pairs was confirmed by Natural bond orbital (NBO) analyses. The protonation of the N2 ligand using decamethyl chromocene (CrCp*2) in the presence of lutidinium salt afforded 1.22 equivalents of ammonia (NH3). Reference[1] Cha, J.; Kwon, H.; Song, H.; Lee, E. Dalton Trans., 2020, 49, 12945–12949



Poster Presentation : **INOR.P-75**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Adsorptive Removal of Radionuclide Cs+ in Water using Acid Active Clay

Keon Sang Ryoo

Department of Applied Chemistry, Andong National University, Korea

Natural white clay was treated with 6 M of H2SO4 and heated at 80oC for 6 h under mechanical stirring and the resulting acid active clay was used as an adsorbent for the removal of Cs+ in water. The physicochemical changes of natural white clay and acid active clay were observed by X-ray Fluorescence Spectrometry (XRF), BET Surface Area Analyser and Energy Dispersive X-line Spectrometer(EDX). While activating natural white clay with acid, the part of Al2O3, CaO, MgO, SO3 and Fe2O3 was dissolved firstly from the crystal lattice, which bring about the increase in the specific surface area and the pore volume as well as active sites. The specific surface area and the pore volume of acid active clay were roughly twice as high compared with natural white clay. The adsorption of Cs+ on acid active clay was increased rapidly within 1 min and reached equilibrium at 60 min. At 25 mg L- of Cs+ concentration, 96.88% of adsorption capacity was accomplished by acid active clay. The adsorption data of Cs+ were fitted to the adsorption isotherm and kinetic models. It was found that Langmuir isotherm was described well to the adsorption behavior of Cs+ on acid activae clay rather than Freundlich isotherm. For adsorption Cs+ on acid active clay, the Langmuir isotherm coefficients, Q, was found to be 10.52 mg g-1. In acid active clay/water system, the pseudo-second-order kinetic model was more suitable for adsorption of Cs+ than the pseudo-first-order kinetic model owing to the higher correlation coefficient R2 and the more proximity value of the experimental value qe,exp and the calculated value qe,cal. The overall results of study showed that acid active clay could be used as an efficient adsorbent for the removal of Cs+ from water.

Poster Presentation : **INOR.P-76**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Comparison of natural white clay and acid-activated white clay for removal of Cd(II) ion from aqueous solution

Keon Sang Ryoo

Department of Applied Chemistry, Andong National University, Korea

Natural white clay obtained from Pohang city in Korea was treated with 6 M H2SO4 and heated at 90oC for 8 h. The generated clay, called as acid-activated white clay in this study, was employed as an adsorbent for the removal of Cd2+ in aqueous solution. It was found that the specific surface area and the pore volume of acid-activated white clay were enhanced when compared with those of natural white clay. The adsorption rate of acid-activated white clay towards Cd2+ occurred steeply at initial contact time and reached equilibrium within 0.5 h. The amount of Cd2+ adsorbed at equilibrium reduced from 94.2 % to 37.94 % by increasing initial Cd2+ concentrations from 10 mg L-1 to 100 mg L-1, whereas the amount of Cd2+ increased from 13.54 % to 93.38 % as adsorbent dose increases from 0.1 g to 1.0 g. The adsorption data of Cd2+ by acid-activated white clay were introduced to pseudo-first-order and pseudo-second-order kinetics, and Freundlich and Langmuir adsorption isotherms, respectively. It was seen that the pseudo-second-order kinetics and the Langmuir isotherms were applied well to describe the adsorption behavior of acid-activated white clay towards Cd2+ due to their higher correlation coefficient R2. The maximum adsorption capacities of Langmuir, Q, for natural white clay and acid-activated white clay were found to be 17.15 mg g-1 and 36.48 mg g-1, respectively. The results of study suggest that acid-activated white clay can be used as an efficient and low-cost material for the removal of Cd2+ from wastewater.

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Poster Presentation : **INOR.P-77**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Study on the Morphological Change and Reduction of Nitrogen and Phosphorous in Litter and Compost of Cowshed

Keon Sang Ryoo

Department of Applied Chemistry, Andong National University, Korea

Litter and compost were obtained at a cowshed of a livestock farm in Andong city in Korea. We examined the morphological change of nitrogen and phosphorous from these samples and tried to suggest a more useful and realistic way for reducing them. Constituents and their content of sample were identified by XRF. NO2-, NO3-, PO43- and NH4+, T-P, T-N released from sample were analyzed using ion chromatograph and UV/Vis spectrometry, respectively. As the results of this study, the ammonia in the early stage of cow excretion is a need to make an ammonia gas state that can be immediately volatile by increasing the pH. Nitrogen and phosphorous, the main source of nutrition in green algal bloom can be reduced by transforming insoluble salts such as calcium phosphate (CaHPO4·3H2O) and struvite (NH4MgPO4·6H2O), respectively, with addition of Ca and Mg after stimulating fermentation of compost.

Poster Presentation : **INOR.P-78**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Fermentation Efficiency and Effect on Morphological Change of Nitrogen and Phosphorous by the Litter Types of Cowshed

Keon Sang Ryoo

Department of Applied Chemistry, Andong National University, Korea

The manure made of chaff and sawdust as litter was collected separately at a cowshed of a livestock farm in Andondg city. The fermentation efficiency of excreta is greatly influenced by the type and characteristics of litter and a factor to be considered for reducing N and P, the causes of eutrophication. Changes in weight with temperature and constituents of sample were examined using TG-DTA and XRF, respectively. NO2-, NO3-, and PO43- ions and NH4+, T-P and T-N eluted from manure by rain were analyzed using ion chromatograph and UV/Vis spectrometry, respectively. As a result, the fermentation efficiency of excreta in sawdust manure is three times higher as compared with chaff manure. The higher the fermentation efficiency, ammonia nitrogen was highly de-nitrogenated and organic phosphorous were also changed into phosphorous ions. Furthermore, phosphorous ions can be removed by transforming insoluble salts such as calcium phosphate (CaHPO4·3H2O) and struvite (NH4MgPO4·6H2O) with addition of Ca and Mg.

Poster Presentation : **INOR.P-79**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Noble Metal-Based Bimetallic Alloy Nanocrystals in Mesoporous Silica for Catalytic Applications

Eunseo Hong, Won Seok Seo*

Department of Chemistry, Sogang University, Korea

Noble metal-based bimetallic alloy nanocrystals have been widely used as heterogeneous catalysts for various hydrogenation reactions of organic compounds because they offer high efficiency and selectivity in molecular hydrogen activation. Herein, we prepared nano-sized bimetallic alloys composed of a noble metal and a first-row transition metal in mesoporous silica. In addition, we controlled the metal-shell thickness of the bimetallic alloy nanocrystals using different HCl concentrations, thereby etching the surface transition metal atoms. The resulting nanocrystals were characterized by XRD, TEM and EDX. These catalysts show an excellent catalytic performance for hydrogenation reactions of organic compounds at relatively mild condition. We demonstrated that catalytic activities of noble metals could be improved by introducing first-row transition metals via promoting the electronic interaction between noble metals and transition metals.

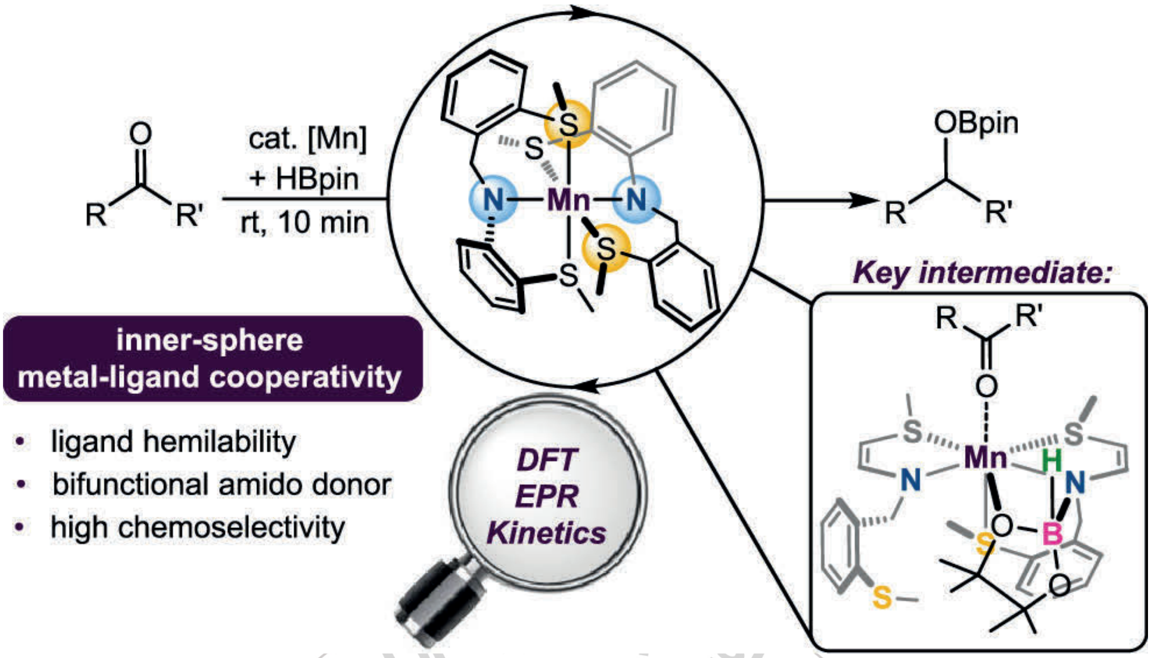
Poster Presentation : **INOR.P-80**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mn(II)-catalyzed Hydroboration with an SNS Ligand: A Metal Hydride-Free Pathway with Metal-Ligand Cooperativity in Action

Mina Son, Matthew R. Elsby[1], Jessica Martin[1], Mu-Hyun Baik[*], R. Tom Baker[1,*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Chemistry and Biomolecular Sciences and Centre for Catalysis Research and Innovation, University of Ottawa, Canada*

Metal-ligand cooperativity (MLC), in conjunction with first-row metal centers has made possible a number of interesting catalytic transformations. Herein, we report a Mn(II) complex bearing a [$S^{Me}NS^{Me}$] ligand catalyzing hydroboration of carbonyls with MLC. The reaction proceeds at room temperature with low catalyst loadings of 0.1 mol % and fast reaction time of 30 minutes.Mechanistic studies via both experimental and computational methods were conducted. Results suggest that a Mn–H intermediate, commonly proposed for Mn-catalyzed hydroboration reactions, is not responsible for catalysis. Alternatively, the amide moiety on the ligand scaffold activates the B–H bond and an outer-sphere hydroboration mechanism is suggested. The hemilability of the thioether moiety is critical for providing a vacant coordination site. Also, the saturation around the metal center is suggested as a reason for favoring the outer-sphere pathway.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ligand hemilability
bifunctional amido donor
high chemoselectivity
DFT
EPR
Kinetics

Poster Presentation : **INOR.P-81**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Influence of Biomolecules on the Activity of Matrix Metalloproteinase-9

Hang Choi, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

Matrix metalloproteinases (MMPs) have been proposed as pathological indicators for various diseases including Alzheimer’s disease (AD), intervertebral disc degeneration, and restenosis. Among MMP family, MMP-9 has been revealed to be associated with AD because its increased level was observed in the brain tissue of AD patients. In addition, MMP-9 degrades both amyloid precursor protein (APP) and amyloid-β (Aβ) which could form toxic aggregates causing AD. In this study, we will examine the influence of multiple natural products (e.g., vitamins) on MMPs’ peptide degrading ability as well as propose the mechanisms how those biomolecules affect the activity of MMPs under various conditions (e.g., stoichiometry) using biochemical and biophysical methods (i.e., zymography, colorimetric assay, docking simulations). Our overall investigation from multiple experiments could provide better insight into the study of the MMP-9 which could cleave Aβ, related to AD pathology.

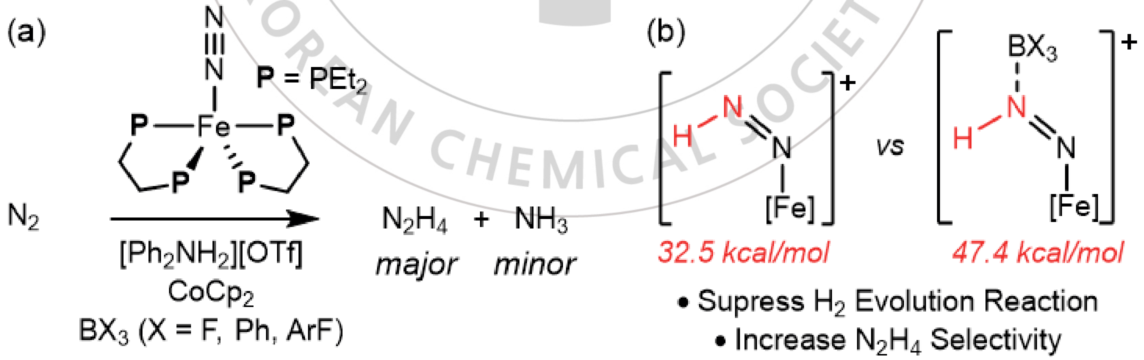
Poster Presentation : **INOR.P-82**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Lewis Acid-Promoted Selective and Efficient Synthesis of Hydrazine

Seongyeon Kwon, **Mu-Hyun Baik**[*]

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

Dinitrogen is the most prevalent feedstock in the atmosphere, yet its conversion to valuable products is challenging due to an inert reactivity. Hydrazine is one of the potential products generated through the hydrogenation of dinitrogen, while only a few catalysts are known to afford it selectively.Fe-based selective hydrazine formation with high acid/reductant loading was reported by Ashley group. To investigate the origin of selectivity, density functional theory calculations are carried out. Theoretical investigation reveals that the stability of intermediates is a key factor determining the performance of Fe catalyst. Based on an elaborate design of steric and electrostatic features of Lewis acids, we propose a simple and effective Lewis acid-catalyzed nitrogen reduction increasing the selectivity and turnover of hydrazine.



Poster Presentation : **INOR.P-83**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Photocatalytic CO_2 Reduction by Half-Metallocene Ruthenium(II) Catalyst and Its Mechanistic Investigation

Daehan Lee, Min Su Choe, Yunjeong Seo, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

This study details the photocatalytic CO_2-to-CO or formate conversion activities of two different photocatalytic systems (IrPE + **(*p*-Cym)RuPE** and IrP/TiO_2/**(*p*-Cym)RuP**) to evaluate the catalytic behavior of homogeneous and heterogenized (*p*-Cym)Ru(II) catalyst, respectively. A single run photolysis of the mixed homogeneous system (IrPE + **(*p*-Cym)RuPE**) in the presence of 16.7 vol % TEOA exhibited a maximal turnover number (TON) of ~800 for 48 h with a high product selectivity of formate (>79%), while the ternary hybrid system with TiO_2-immobilized **(*p*-Cym)RuP** showed the relatively higher and steady CO_2-to-CO and CO_2-to-formate conversion activities (a TON of >1660 for 100 h), reflecting the CO_2 reduction route bisected by heterogenization of **(*p*-Cym)RuP**. The mechanistic investigations along with photophysical and electrochemical studies suggest that the occurrence of MLCT ((*p*-Cym)Ru^{I}(bpy)$]^{+}$ → [(*p*-Cym)Ru^{II}($bpy^{\bullet -}$)$]^{+}$) onto the electron-withdrawing n-type TiO_2 opens catalytic route toward (*p*-Cym)Ru^{II}-COOH intermediate that results in CO_2-to-CO conversion, apart from the typical catalytic route via (*p*-Cym)Ru^{II}–H intermediate for formate production.

Poster Presentation : **INOR.P-84**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Optical responses of polymer-grafted anisotropic gold nanoparticles in different dimensional factors

Jaedeok Lee, Juyeong Kim*

Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University,
Jinju 52828, Korea

Noble metal nanoparticles have plasmonic properties that can be highly sensitive to local changes in dielectric environment. In particular, polymer-grafted metal nanoparticles have shown active response to external stimuli. We prepared anisotropic gold nanoparticles with various edge lengths, and they could be grafted by polystyrene layers with different thicknesses. Such polymer-grafted gold nanoparticles were characterized by UV-visible spectroscopy, quantitative image analysis, and finite-difference time-domain simulations. We found that the spectral shift for localized surface plasmon resonance (LSPR) depended on the core size, shape, and polymer thickness. In addition, the polymer-grafted gold concave cube showed a larger LSPR spectral shift than the cubic shape, indicating higher sensitivity to temperature changes. Our research will not only provide systematic insight into the optical properties of polymer-grafted gold nanoparticles, but also help design stimuli-responsive plasmonic sensors.

Poster Presentation : **INOR.P-85**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Potent Application of Vermicide and Vitamins as regulators of the Activity of Neprilysin

Hang Choi, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

Neprilysin (NEP) is a zinc metalloproteinase that has been suggested to be involved in several diseases such as Alzheimer's disease (AD), and heart failure (HF). NEP could degrade amyloid-β (Aβ) which could be related to the pathology of AD. Moreover, NEP is considered to lead natriuretic peptides become inactive and consequently, the occurrence of HF. Thus, the regulation of NEP could be an important point to improve the understanding of AD pathology and curing HF. From previous studies, most of NEP regulators have common structure , phenyl residue, such as polyphenols (e.g., caffeine). Recently, well known vermicides, Albendazole and Mebendazole, have been suggested to be potent anti-cancer drugs. In addition, they have structural similarity to NEP regulators indicating that they could have possibility to control the activity of NEP. Therefore, in this study, we will determine whether both Albendazole and Mebendazole could act as NEP regulators by biophysical and biochemical experiments mass spectrometry, ELISA, enzyme activity assays, and Western blot.

Poster Presentation : **INOR.P-86**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Purification of Sodium Pentazolate as Polynitrogenic Compounds

Hae-Wook Yoo[*], Kuktae Kwon, SeungHee Kim, So Jung Lee

Agency for Defense Development, Korea

Nitrogen rich compounds are very important materials in the field of high-energy material development. In general, since nitrogen exists in a very stable diatomic molecule of tripe bonds (N≡N, 228 kcal/mol), it is possible to release large energy through the decomposition process of nitrogen rich compounds including nitrogen of single (N-N, 39 kcal/mol) or double bonds (N=N, 100 kcal/mol). Ultimately, if polynitrogen composed of only nitrogen exists, it is predicted having a significantly higher energy density compared to the conventionally developed explosives will be possible, so efforts to develop polynitrogen have been continuously made. After the research results on the synthesis of pentazinium (N_5^+) were published in 1999, they received a lot of attention, but no progress was made. In 2017, pentazolate compounds (cyclo-N_5^-) was synthesized in lab-scale, interest in polynitrogen is growing again. In this study, we synthesized and confirmed the presence of pentazolate compound by high-resolution mass spectrometer. In addition, in previous studies, purification was carried out using the chromatography method, but due to limitations in application when increasing the amount of synthesis, purification using the filtration method was attempted and appropriate results were abtained.

Poster Presentation : **INOR.P-87**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Photosensitization Process of Organic Donor-*π*-Acceptor Dye in CO_2 Reduction by Re(I)-Complex-immobilized TiO_2 Hybrid Catalyst

Min Su Choe, Sanghun Lee, Daehan Lee, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

In this study, we have finely tailored a metal-free organic dye in photocatalytic CO_2 reduction system prepared by fixing a dye and a Re(I) complex on TiO_2 nanoparticles. In series of dyes, **Flu-CNCA**-sensitized TiO_2/ReP particles exhibited the most efficient CO_2 to CO conversion activity (a TONCO of ~1089 for >70 h) with 3 vol % H_2O in DMF solution; irradiation at λ >400 nm. Under irradiation at λ > 500 nm, the hybrid ternary system using *π*-extended dye showed more than 5 times higher CO_2 to CO conversion activity than conventional organic dye.

Poster Presentation : **INOR.P-88**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Selective CO_2-to-Formate Conversion Triggered by Effective Proton Shuttle of Pendant Brønsted Acid/Base Sites in the Photochemical CO_2 Reduction by Mono-Bipyridyl Ru(II) Catalysts

Yunjeong Seo, Daehan Lee, Min Su Choe, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

While the incorporation of pendant Brønsted acid/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. Herein, we report two new *trans*(Cl)-[Ru(6-X-bpy)$(CO)_2Cl_2$] complexes functionalized with saturated ethylene-linked functional group (bpy = 2,2′-bipyridine; X = $–(CH_2)_2–OH$ or $–(CH_2)_2–N(CH_3)_2$) at the *ortho*(6)-position of bpy ligand, which are named **Ru-bpy^{OH}** and **Ru-bpy^{diMeN}**, respectively. In the series of photolysis experiments, compared to non-tethered 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. From a series of in situ FTIR analyses, it was found that the Ru-formate intermediates are stabilized by a highly probable hydrogen bonding between pendent proton donors (–diMeN$^+$H or –OH) and the oxygen atom of metal-bound formate (Ru^I–OCHO···H–*E*–$(CH_2)_2$–, *E* = O or diMeN$^+$). Under such conformation, the liberation of formate from the stabilized Ru^I-formate becomes less efficient compared to the non-tethered case, consequently lowering the CO_2-to-formate conversion activities during photoreaction.

Poster Presentation : **INOR.P-89**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Photosensitization Process of Porphyrinic Metal-Organic Frameworks (MOF) in CO_2 Reduction by a Re(I)-complex Doped MOF Hybrid Catalyst

Yunjeong Seo, Daehan Lee, Sanghun Lee, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

A porphyrinic metal-organic framework (**PMOF**) known as PCN-222(Zn) was chemically doped by with the molecular Re(I) catalyst bearing carboxylate anchoring group to form a new type of MOF-Re(I) hybrid photocatalyst. The porphyrinic MOF-sensitized hybrid (**PMOF/Re**) prepared with an archetypical CO2 reduction catalyst, $(L)Re^{I}(CO)_3Cl$ (Re(I); L = 4,4′-dicarboxylic-2,2′-bipyridine), in the presence of 3 vol% water produced CO with no leveling-off tendency for 59 h to give a turnover number of ≥1893 (1,070 ± 80 μmol h^{-1} (g MOF)$^{-1}$). The high catalytic activity arises mainly from efficient exciton migration and funneling from photoexcited porphyrin linkers to the peripheral Re(I) catalytic sites, which is in accordance with the observed fast exciton (energy) migration (≈1 ps) in highly ordered porphyrin photoreceptors and the effective funneling into Re(I) catalytic centers in Re(I)-doped **PMOF** sample. Enhanced catalytic performance is convincingly supported by serial photophysical measurements including decisive Stern-Volmer interpretation.

Poster Presentation : **INOR.P-90**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

MOF-based adsorbents with high stability and reusability for CO_2 capture

Jong Hyeak Choe, Hyojin Kim, Minjung Kang, Hyein Park, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Amine-appended adsorbents can effectively remove CO_2 generated from the post-combustion process. Among these adsorbents, diamine-appended M_2(dobpdc) series show remarkable CO_2 capture. However, diamine-appended Mg_2(dobpdc) have demonstrated low reusability during adsorption-desorption cycles under humid conditions because the coordinated diamines are volatilized and exchanged with H_2O. Therefore, we focus on this problem and tried to increase the reusability under humid conditions. In order to improve recyclability, we reacted diamine-appended Mg_2(dobpdc) with epoxide compounds under mild conditions. The adsorbent, which is combined with epoxide, exhibited high contact angle of a water droplet and low water vapor capacity. Furthermore, it showed a good recyclability under humid CO_2 conditions. More details can be found on the poster.

Poster Presentation : **INOR.P-91**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Control of Metal Composition in a Multimetallic Metal-Organic Framework via Mechanochemical Formation

Hyojin Kim, Minjung Kang, Jong Hyeak Choe, Hyein Park, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Multimetallic metal-organic frameworks (MOFs) have received considerable interests due to their potential of enhanced activities for gas sorption and separation, and catalysis. Herein, we demonstrate a synthetic strategy through mechanochemical formation for controllable metal composition in the multimetallic MOF. A controlled stoichiometric composition of metal nodes in the MOF system was achieved, as confirmed by TEM-EDS, elemental analysis, and ICP-AES. Moreover, additional characterizations including powder x-ray diffraction, infrared spectroscopy, X-ray photoelectron spectroscopy, and gas sorption are carried out to confirm the successful formation and pore environment. Detailed synthetic scheme and characterization will be presented in the poster.

Poster Presentation : **INOR.P-92**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Hyper-crosslinked polymers for ethane/ethylene separation

Hyein Park, Minjung Kang, Jong Hyeak Choe, Hyojin Kim, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

The separation of ethane from ethylene is important in the production of polymer-grade ethylene for industrial manufacturing. We synthesized hyper-crosslinked polymers (HCPs) and evaluated their ethane selectivity over ethylene. These polymers exhibit the preferential adsorption of ethane over ethylene and showed high adsorption capacity of ethane at 1 bar. The separation performance of HCPs for ethane/ethylene separation was confirmed by gas adsorption isotherms, ideal adsorbed solution theory (IAST) calculations, and experimental breakthrough curves. Detailed synthetic scheme and specific properties will be presented in the poster.

Poster Presentation : **INOR.P-93**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Double Post-Synthetic Modifications of Robust Metal-Organic Framework for Enhanced Gravimetric and Volumetric Ammonia Capacity

Daewon Kim, Minjung Kang[1], Chang Seop Hong[1,*]

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

While interest in hydrogen as a green fuel is growing rapidly, the role of ammonia as a hydrogen transporter is in the spotlight due to the high energy density of ammonia compared to hydrogen. Meanwhile, for practical applications volumetric capacity as well as gravimetric capacity must be considered simultaneously. Herein, we reported acidic group functionalized metal-organic frameworks prepared via double post-synthetic modifications showing high gravimetric and volumetric ammonia capacity with facile regeneration. The ammonia storage properties and adsorption mechanism were characterized by ammonia isotherm, NH_3-temperature-programmed desorption curves, NH_3 breakthrough curves, and in-situ FT-IR. Detailed synthesis and properties will be presented in the poster.

Poster Presentation : **INOR.P-94**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Characterizations of 1,1-Dihexyl-2,5-diethynyl-3,4-diphenyl-silole

Se yeon Park, Young Tae Park[1,*], Ji Hun Lee[1], Hyeong Rok Si

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

1,1-Dialkyl (R = Et, or *iso*-Pr, or *n*-Hex)-2,5-dibromo-3,4-diphenyl-siloles were prepared by the reactions of 1,1-dialkyl (R = Et, or *iso*-Pr, or *n*-Hex)-1,1-di(phenylethynyl)silanes with lithium naphthalenide, zinc chloride, and *N*-bromosuccinimide (NBS), respectively. Two bromine groups of the prepared siloles were substituted with two trimethylsilylethynyl groups using trimethylsilylacetylene (TMSA) under the solvent of diisopropylamine and catalysts such as palladium chloride, copper iodide, and triphenylphosphine, of which 1,1-dialkyl(R = Et, or *iso*-Pr, or *n*-Hex)-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles were yielded, respectively. 1,1-Dihexyl-2,5-diethynyl-3,4-diphenyl-silole was only successfully prepared by desilylation reaction of 1,1-dihexyl-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-silole with potassium carbonate (K_2CO_3) and co-solvent of tetrahydrofuran (THF) / methanol. After the reaction was finished, potassium carbonate was removed by washing with dilute HCl aqueous solution. The crude product was extracted with dichloromethane (DCM), and further purified by recrystallization in hexane. The obtained product was soluble in usual organic solvents such as tetrahydrofuran and dichloromethane. All the prepared materials were characterized by ^{1}H, ^{13}C, ^{29}Si NMR, IR, and UV-Vis spectroscopic methods. 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-95**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Electrochemical morphology evolution of copper on single gold nanoparticles

Hyunsik Hwang, Hyunjoon Song*

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

The bimetallic structures are used in various applications such as catalysis and sensors. Bimetallic nanoparticles have different photophysical properties depending on size and components, it is significantly important to study and correlate structural changes with optical properties. Among them, if noble metals are used, changes of metals surface in the reaction conditions could be observed without sophisticated systems because of localized surface plasmon resonance (LSPR). In this study, Au-Cu were constructed using electrochemical methods for improved interface conductivity and fewer surfactants at the liquid-solid interface. The electrochemical synthesis of nanoparticles has been rarely reported with uniform and well-defined shapes. We synthesized well-defined Au-Cu nanostructures using single Au nanoparticles and showed that the morphology of Au-Cu particles was controlled through particle density. As the particle density changes, the growth of Cu domains into cubes, perforated cubes, and octa-pods. In addition, in-situ single-particles scattering spectroscopy was conducted to track the change in plasmonic properties with the growth of bimetallic structures. Finally, a mechanism study was implemented by combining optical information and morphologies. It is expected that this can be applied to nanoparticles with various elements.

Poster Presentation : **INOR.P-96**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Post-synthetic Modification for Cyclization in Metal-Organic Frameworks

Haneul Yoo, Min Kim[1,*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk National University, Korea*

Three-dimensional, porous metal-organic frameworks (MOFs) could have functional groups in their pores, and the chemical property and environment are directly related with functional group of MOFs. For last two decades, various functional groups such as amino, nitro, halo, hydroxy, and additional aromatic rings have been successfully incorporated into MOFs through ligand functionalization. Additionally, the chemical handles in MOFs could be converted to other functionalities in the solid-state manner, which called post-synthetic modification (PSM). Traditional organic transformations have been accomplished through PSM strategy.[1]

Acylation of amines and Click reactions (CuAAC, SuFEx, thiol-ene) were intensively studied, and cyanation, chlorination, and other functional group conversions were introduced in MOFs through PSM manner. In this work, new PSM strategy for cyclization has been investigated. When the MOFs have two reactive sites, the chemical connection between two sites was successfully performed. The detail strategies and characterizations of MOFs will be presented.

Reference1 Kalaj, M.; Cohen, S. M. *ACS Cent. Sci.* **2020**, *6*, 1046.

Poster Presentation : **INOR.P-97**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Electrochemical Properties of 1,1-Dialkyl-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles

Hyeong Rok Si, Young Tae Park[1,*], Ji Hun Lee[1], Se Yeon Park

chemistry department, Keimyung University, Korea
[1]Department of Chemistry, Keimyung University, Korea

1,1-Dialkyl (ethyl, or *iso*-propyl, or *n*-hexyl)-2,5-dibromo-3,4-diphenyl-siloles were prepared by the reactions of 1,1-dialkyl (ethyl, or *iso*-propyl, or *n*-hexyl)-1,1-di(phenylethynyl)silanes with lithium naphthalenide, $ZnCl_2$, and *N*-bromosuccinimide (NBS), respectively. Two bromine groups of the prepared siloles were replaced 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 (ethyl, or *iso*-propyl, or *n*-hexyl)-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles were yielded, respectively. The photochemical properties, such as UV-Vis absorption, excitation, and fluorescence emission spectra, of the prepared materials were investigated. Each coin cell was made with the three synthesized silole materials, and their lithium-ion battery properties, for example, cyclic voltammetry (CV), C-rate performance, cycling performance, and electrochemical impedance spectroscopy (EIS) were also studied, in particular. Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2020R1I1A3A04036901).

Poster Presentation : **INOR.P-98**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Quaternary Ammonium Group Installations into Zr-based Metal-Organic Frameworks

HoJeong Choi, Seungpyo Hong[1], Min Kim[*]

Department of Chemistry, Chungbuk National University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Derivatizations with functional groups are recognized as an important feature of metal-organic frameworks. Various organic functional groups have introduced in MOFs such as amino, hydroxy, halo, alkoxy groups, and etc. Among them, the amino group was widely studied due to tolerance toward MOF synthetic condition, unique basicity, and good reactivities. A series of amino group derivatives were successfully studied in MOFs.[1]

Zr-based MOFs have been extensively investigated and applied in various research fields due to high chemical and physical stabilities. The most well-known Zr-based MOF, UiO-66 (UiO = University of Oslo) series are stable even in aqueous conditions. However, due to the strong Lewis acidic character of zirconium cation and C-N bond cleavages, the amine derivatization and the direct ammonium group installation were not fully investiaged.[2]

In this presentation, our recent result for ammonium group installation in Zr-based UiO-66 MOFs will be presented. Both aromatic ammonium and aliphatic ammonium groups were studied, and both direct alkylation and Click chemistry were investigated. The strategical approaches and MOF characterizations will be discussed.

References1. Lin, Y.; Kong, C.; Chen, L. *RSC Adv.* **2016**, *6*, 32598.2. Hahm, H.; Ha, H.; Kim, S.; Jung, B.; Park, M. H.; Kim, Y.; Heo, J.; Kim, M. *CrystEngComm*, **2016**, *17*, 5644.

Poster Presentation : **INOR.P-99**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Strategy on the Preparation of Tetrazole-Functionalized Metal-Organic Frameworks

Sangho Lee, Lee Daeyeon[1], Jun Yeong Kim[2], Seungheon Cha[2], Jooyeon Lee[3], Min Kim[3,*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]Chemistry, Chungbuk Natioanl University, Korea
[2]Chungbuk Natioanl University, Korea
[3]Department of Chemistry, Chungbuk National University, Korea

Tetrazole is five-membered heterocyclic compound with single carbon and four nitrogen atoms. Simple tetrazole generally has one alkyl substituent on carbon and one free NH bond among four nitrogen atoms. This proton shows high acidity like carboxylic acid due to the delocalized structures between tetrazolate.[1]

Due to the strong metal coordinating ability of tetrazolate like carboxylates, various metal-organic frameworks (MOFs) syntheses with tetrazole-containing organic ligands have been extensively studied. [2] Zinc, Co, Mn, Cd, and Fe-based MOFs were mainly studied with tetrazolate ligands, in addition, Cr, Ni, Ag, and Hg were reported for MOF with metal-tetrazolate coordination.

In this work, a new strategy for introducing free-tetrazole group into MOFs has been investigated. In specific, a tetrazole-functionalized, which means containing free-tetrazole-tethered, Zr-based MOF synthesis was attempted. Direct synthesis with target ligand and post-synthetic modification (PSM) toward tetrazole strategies will be discussed with characterization data.

References1. Satchell, J. F., Smith, B. J. *Phys. Chem. Chem. Phys*. **2002**, *4*, 4314.2. Tabacaru, A.; Pittinari, C. Galli, S. *Coord. Chem. Rev*. **2018**, *372*, 1.

Poster Presentation : **INOR.P-100**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Extremely Active Ethylene Tetramerization Catalyst Synthesis using PNP framework $[iPrN(PAr_2)_2\text{-}CrCl_2]+[B(C_6F_5)_4]–$ (Ar = $-C_6H_4$- *p*-SiR_3)

JungHyun Lee, Bun Yeoul Lee[*]

Department of Molecular Science and Technology, Ajou University, Korea

In the early 2000s, Sasol discovered Cr based selective ethylene tetramerization catalyst. After this lots of attempt have been made to develop “on-purpose” 1-octene production technology. We prepared a series of bis(phosphine) ligands containing bulky $–SiR_3$ substituents, and found an extremely active catalyst to meet the standard for commercial . All the Cr complexes obtained by reacting ligands with $[(CH_3CN)_4CrCl_2]^+[B(C_6F_5)_4]^-$ (i.e., $[iPrN(PAr_2)_2CrCl_2]^+[B(C_6F_5)_4]^-$) exhibited high activity exceeding 6000 kg/g-Cr/h when combined with inexpensive iBu_3Al avoiding the use of expensive MMAO (modified-methylaluminoxane). Bulky $–SiR_3$ substituents played a key role in the success, blocking formation of inactive species (Cr complex coordinated by two $iPrN(PAr_2)_2$ ligands, i.e., $[(iPrN(PAr_2)_2)_2\text{-}CrCl_2]^+[B(C_6F_5)_4]^-$). Among the prepared catalysts, [**3** $-CrCl_2]^+[B(C_6F_5)_4]^-$ showed the highest activity (11,100 kg/g-Cr/h, 100 kg/g-catalyst) with high 1-octene selectivity (75 wt%), furthermore reducing generation of undesired >C10 fraction (10.7 wt%). A 10-g scale synthesis of **3** as well as a convenient and low-cost synthetic method for $[(CH_3CN)_4CrCl_2]^+[B(C_6F_5)_4]^-$ were developed.

Poster Presentation : **INOR.P-101**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Covalent Functionalization of Metal-Graphite Core-Shell Nanocrystals

Jisoo Jung, Won Seok Seo*

Department of Chemistry, Sogang University, Korea

We have synthesized highly uniform, ultra-small (mostly 2 to 4 nm) metal/graphitic carbon shell (Metal/GC) nanoparticles by thermal decomposition of metal precursors in ordered mesoporous silica and subsequent methane chemical vapor deposition (CVD). The Metal/GC nanoparticles have been covalently functionalized via chemical reactions between graphite and organic compounds. The functionalized Metal/GC nanoparticles are soluble and stable in water solutions. The nanoparticles have been characterized by UV-vis, XRD, DLS, TEM, and IR. We expect the functionalized FeCo/GC nanoparticles to be useful for biomedical applications including magnetic cell separation, bio-detection, and magnetic-resonance imaging.

Poster Presentation : **INOR.P-102**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Selective synthesis of Iridium Supramolecules by Precise Control of Binding/Chelating Modes of Tetrazolyl Ligands

Guitae Park, Junseong Lee[1,*]

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

In the field of coordination chemistry, a variety of mono-, di-or tri-tetrazolyl systems have been used as linkers for the complexation. This is because dative coordination bonding between metal center and electron donor has provided an efficient strategy to construct designated supramolecular architecture. However, compared with well-known pyridine and imidazole systems, tetrazole have not been used extensively in the supramolecular chemistry in spite of its versatile coordination modes. Also, while several reports concern the control of chelating/bridging modes in the complexation, there is no report on the precise control in chelating/bridging modes in the tetrazolyl ligands to our knowledge. Therefore, it will be interesting if we can control the binding modes or shapes of electron donor units easily for the precise structural tuning of the desired supramolecules. Herein, we report the selective formation of multinuclear Ir supramolecules by controlling structural factors of tetrazolyl units.

Poster Presentation : **INOR.P-103**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Structural study through 1-D Zinc Tetrazole Coordination Polymer synthesis

Ga Hee Noh, Junseong Lee*

Department of Chemistry, Chonnam National University, Korea

Tris(pyrazolyl)borates complex, called as ‘scorpionate’, is a tridentate ligand system and considered as a quite useful tridentate ligand. It occupied one facial site and acted quite similarly with cyclopentadienyl ligand, providing broad applications in the field of supramolecular assembly, catalysis, and enzyme modeling. Despite the design similarities, strongly donating scorpionates differ in their topology and flexibility, donor properties and degradation pathways. The structural and electronic properties of these ligands are contrasted and related to their chemistry, particularly that of the transition metals. Recently, we reported metallascorpionate system possessing Fe metal center and hydroxyphenyl tetrazole (TzPhOH) and its additional coordination behavior toward alkali metal ions such as Li, Na, K. It has two different binding sites (κ3-O3, κ 3-N3), resulting in the sandwich-like formation with the sequence of K–FeTz3–K. Moreover, by the addition of zinc perchlorate, trimetallic coordination porous material was achieved. In the compound, one-dimensional hetero-tri-metallic ions array of with the sequence of (-K-K-K-Fe-Zn-Fe-). To extend the library of metallascorpionate system, simple reaction of metal perchlorate and TzPhOH was conducted in the presence of potassium hydroxide. Interestingly, high dimensional zinc coordination polymer was achieved and its structure was confirmed by X-ray crystallography. In the structure, unprecedented one-dimensional zinc ions array was observed. In this presentation, the detailed synthesis and characterization of the 1-D zinc coordination polymer is discussed. The ability of strongly donating scorpionate ligands to stabilize metal ligand multiple bonds in late transition metal complexes is also briefly discussed.

Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Effects of Impurity and Functionalized Ligands on Ag Nanoparticles Embedment into Ligand Functionalized Silica Gels

Jeong Woo Hong, Hee-Jung Im[*]

Department of Chemistry, Jeju National University, Korea

Ag nanoparticle-embedded ligand functionalized silica gels were prepared for the investigation of impurity and functionalized ligands effects on the embedment of Ag nanoparticles in ligand functionalized mesoporous silica gels. Ag nanoparticle solutions with and without surfactant were prepared referring to previously published papers. After that, commercial ligand functionalized silica gels were added into the solutions and then stirred for 18 hours at room temperature in the dark. Ag^+ ion coated ligand functionalized silica gels without using a reducing agent were also prepared to be compared with Ag nanoparticle-embedded ligand functionalized silica gels. The prepared Ag nanoparticle-embedded and Ag^+ ion coated ligand functionalized silica gels were ready to test after filtering, washing, and vacuum drying.Various spectroscopic analyses were performed to characterize the remaining surfactant and Ag nanoparticles, which are not included in the silica gels. The tendency of Ag nanoparticles to be embedded in ligand functionalized silica gels was clearly different depending on the presence or absence of surfactant and the type of functionalized ligands.

Poster Presentation : **INOR.P-105**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Stable Nickel Monocarbonyl Species Related to the CO Coordination at the Nickel Site of CODH

Yunho Lee[*], Kunwoo Lee[1]

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

Transition metal carbonyl species are found in few metalloenzymes, such as hydrogenases, acetyl-CoA synthase and carbon monoxide dehydrogenases (CODH). In particular, CO coordination and its reversible conversion to CO_2 occurs at the nickel site of CODH. Thus, the chemistry of four-coordinate nickel monocarbonyl species is of our particular interest. A series of nickel carbonyl complexes supported by tridentate pincer ligands such as PNP (PNP^- = bis(2-(diisopropylphosphino)-4-methylphenyl)amide), ^{acri}PNP ($^{acri}PNP^-$ = 4,5-bis(diisopropylphosphino) -2,7,9,9-tetramethyl-9H-acridin-10-ide) and $PP^{Me}P$ ($PP^{Me}P$ = bis(2-(diisopropylphosphinophenyl))-methylphosphine) were synthesized to explore their redox chemistry as well as reactivity towards CO_2. Unlike the nickel monocarbonyl species supported by bisphosphino amido ligands, the CO substitution of $(PP^{Me}P)NiCO$ with CO_2 was not observed. Single crystal X-ray diffraction studies reveal that there are noticeable structural differences between nickel species of both anionic PNP ligands and a neutral $PP^{Me}P$ ligand, which may affect the tendency of CO_2 reactivity. One of the major differences is the ligand planarity. The ^{acri}PNP ligand prefers a planar structure, but the $PP^{Me}P$ ligand favors a distorted geometry such as tetrahedral, when a metal ion binds to it. According to the computational energy calculations, the substitution of a CO ligand by CO_2 in $(PP^{Me}P)NiCO$ to give $(PP^{Me}P)Ni(\mu\text{-}CO_2)$ is thermodynamically unfavorable by +22.64 kcal•mol^{-1}, but the substitution of the nickel monocarbonyl species supported by bisphosphino amido ligands is favorable (PNP^-; −1.7 kcal•mol^{-1} and $^{acri}PNP^-$; −2.16 kcal•mol^{-1} in tetrahydrofuran). To investigate the oxidative reactivity of $(PP^{Me}P)NiCO$, the reactions of $(PP^{Me}P)Ni(\mu\text{-}CO_2)$ with O_2 and ROOH were explored. Upon addition of O_2(g) to the $(PP^{Me}P)NiCO$ solution in toluene at −15 °C, a new intermediate was observed monitored by UV-Vis spectroscopy. Product analysis and related reactions relevant to the reactivity of the nickel site of CODH will be discussed.

Poster Presentation : **INOR.P-106**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Nickel coated rhenium oxide catalyst for hydrazine decomposition to evolve hydrogen gas

Gyeong Eun Hyun, Seok Min Yoon*

Department of Chemistry, Wonkwang University, Korea

Rhenium (Re) has been used as a mechanically substantial component to make jet engines due to their extremely high mechanical stability, when it forms superalloy with other metals. Also, the Re has been fascinated to utilize as a catalyst for olefin metathesis and hydrogenation. Practically, Re-Ni alloy is a widespread catalyst used in the petroleum refinery process. Nevertheless, in academia, the heterogeneous catalytic potential of the Re is still not studied well. Thus, to discover heterogeneous catalytic performance of the Re, we tried to apply synthesized new Ni coated Re-oxides (Ni@ReO$_x$) as an efficient catalyst for decomposing hydrazine ($N_2H_4 \cdot H_2O$) to produce hydrogen (H_2) gas. Hydrazine can be a promising hydrogen fuel due to its high hydrogen content 12.5wt% and easy transportation and storage. Further, it is known that Re catalyst are very resistant to chemical poisoning from nitrogen, so Re can be a sustainable catalyst to decompose the hydrazine and producing H_2 gas from it. Ni@ReO$_x$ catalyst were synthesized by simple solvothermal methods. The Ni@ReO$_x$ were synthesized as crystallites with cube-shaped morphology and their oxidation states were controlled by annealing temperature. The optimized Ni@ReO$_x$ catalyst for hydrazine decomposition produce H_2 gas with high selectivity (over 90% at least) and with a turnover frequence (TOF) value of 240 h^{-1}.

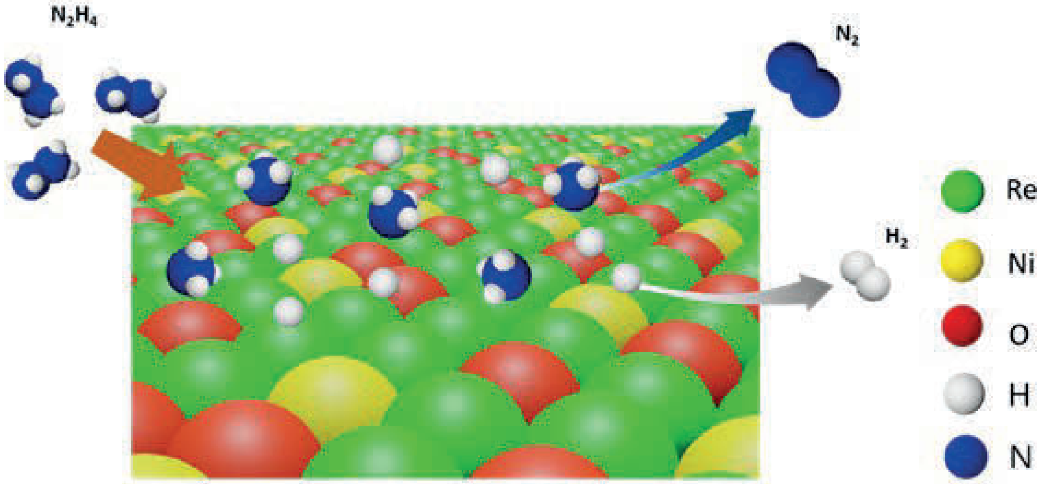


Figure 1. Hydrazien decomposition reaction by transition metal incorporated Ni@ReO_x nanocatalyst.

Poster Presentation : **INOR.P-107**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Ancillary ligand effect on the radiative and non-radiative process in the cyclometalated heteroleptic iridium complex

Daehoon Kim, Kyung-Ryang Wee*

Department of Chemistry, Daegu University, Korea

In the cyclometalated iridium complex, various phenyl pyridine (ppy) type ligand-based homoleptic and heteroleptic Ir complexes were studied and characterized to understand the metal to ligand charge transfer (MLCT). Especially, ppy ligand-based heteroleptic Ir complexes were investigated by many researchers because it's easily controlled the phosphorescent emission color by simple ancillary ligand tuning. Also, it is well known that the emission color tuning of the heteroleptic Ir complexes is originated by the inter-ligand energy (or charge) transfer (ILET) from the main ligand to the ancillary ligand, it means that the emission color tuning limitation is caused by ppy type ligand. In addition, 1-phenyl-1H-pyrazole (ppz) based Ir complex (Ir(ppz)3) is one of the well-known complex but it shows low quantum efficiency in room temperature. Recently, we have reported the ppz ligand incorporated Ir complex, which shows high emission quantum yields more than ppz based Ir complex, but limited information available. In this study, ppz main ligand-based various heteroleptic Ir complexes (**pic**, **Hpic**, **iq**, and **qnx**) including Ir(ppz)3 were designed and successfully prepared to understand the ancillary ligand effect on the radiative and non-radiative process in the ppz type iridium complex. We have employed four different N^O ancillary ligands and the photophysical and electrochemical properties of cyclometalated heteroleptic iridium complex are compared as the structure of the ancillary ligand changes. In the emission spectrum, red-shift was observed in the order of **pic** < **Hpic** < **iq** < **qnx**. In addition, as the polarity of the solvent increases, the properties of red-shift are observed in the emission spectrum.

Poster Presentation : **INOR.P-108**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Cyclometalated N^C Ligand Geometry Isomer Effects in the Pt(II) Complexes for Metal to Ligand Charge Transfer Control

Minjung Chae, Kyung-Ryang Wee[*]

Department of Chemistry, Daegu University, Korea

Three geometry isomers of cyclometalated N^C ligand, consisting *ortho-*, *meta-* and *para*-position linked donor–acceptor structures, were designed and prepared by Suzuki-Miyaura coupling reactions and successfully introduce Pt(II) metal to the three isomers to understand geometry isomer effects on the metal to ligand charge transfer character. Based on the previous our research, the intramolecular charge transfer characters depending on terphenyl geometric isomer effects were studied to confirm the excited state and emission origin. In this study, we have investigated the geometric effect of *ortho*-(**O**), *meta*-(**M**) and *para*-(**P**) terphenyl isomer structure on the Platinum(Pt) complex. The photophysical properties of the terphenyl backbone based **O**, **M** and **P** complexes were compared each other. In the steady state absorption spectra, a little red-shifted property was observed in the order of **O** < **P** < **M** and absorption maximum of near 310 nm correspond to ligand-centered absorption and singlet metal to ligand charge transfer absorption at around ~350 nm. In particular, the emission spectra of the all of complexes showed similar emission maximum of 525 nm, indicated triplet metal to ligand charge transfer emission and it show no significant bathochromic shift. Also, due to the Pt(II) four coordinate square planar structure, three Pt complexes were showed characteristic concentration dependent emission spectra, due to intermolecular interactions. From the experimental results, we confirmed that **P** complex is flat more than **O** and **M** complexes, so **P** complex is more favorable intermolecular interaction in solid state.

Poster Presentation : **INOR.P-109**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Ultrafast excited state relaxation dynamics in a heteroleptic Ir(III) complex, *fac*-Ir(ppy)$_2$(ppz), revealed by femtosecond X-ray transient absorption spectroscopy

Kyung-Ryang Wee*, Mina Ahn

Department of Chemistry, Daegu University, Korea

A typical metal complex has a central metal surrounded by multiple ligands, which greatly affect the properties of the whole complex. Although heteroleptic complexes often exhibit substantially different behaviors from homoleptic complexes, systematic studies to explain their origins have been rare. Of special importance is to understand why the heteroleptic metal complex shows a more complicated excited state relaxation dynamics than the homoleptic metal complex. To address this issue, we investigated the excited state relaxation dynamics of a heteroleptic Ir(III) complex, *fac*-Ir(ppy)$_2$(ppz), and two homoleptic Ir(III) complexes, *fac*-Ir(ppy)$_3$ and *fac*-Ir(ppz)$_3$, using femtosecond X-ray transient absorption (fs-XTA) spectroscopy, ultrafast optical transient absorption (TA) spectroscopy, and DFT/TDDFT calculation. The data show that the ultrafast relaxation dynamics of ~450 fs, which is significantly faster than those of previous Ir(III) complexes with other ligands, is observed only in *fac*-Ir(ppy)$_2$(ppz) but not in the homoleptic Ir(III) complexes. Such dynamics observed for only heteroleptic Ir(III) complexes must originate from the heteroleptic character, and naturally, the inter-ligand energy transfer between two different types of ligands has been suggested to explain the fast dynamics. Both fs-XTA and TA data, however, favor the assignment of the ultrafast dynamics of ~450 fs to the internal conversion (IC) process from the ppz-localized ^{3}MLCT to the ppy-localized ^{3}MLCT. The DFT/TDDFT calculations support that the abnormally fast IC for *fac*-Ir(ppy)$_2$(ppz) is due to a large nonadiabatic coupling and the small energy gap between the two states.

Poster Presentation : **INOR.P-110**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Inter-ligand energy transfer (ILET) process in an Ir-complex with expanding π-conjugated ligand

Mina Ahn, Kyung-Ryang Wee*

Department of Chemistry, Daegu University, Korea

The ILET process in heteroleptic iridium complex, **$[\mathrm{Ir(dfppy)_2(bpy\text{-}Im2)}]^+$** was investigated using a femtosecond transient absorption spectroscopic technique. The photophysical properties of **$[\mathrm{Ir(dfppy)_2(bpy\text{-}Im2)}]^+$** with significantly expanding π-conjugated ligand were compared to those of **$[\mathrm{Ir(dfppy)_2(bpy)}]^+$** and a free **bpy-Im2** ligand. The emission spectrum of **$[\mathrm{Ir(dfppy)_2(bpy\text{-}Im2)}]^+$** showed no shift upon changing the solvent polarity, whereas the free ligand **bpy-Im2** showed the bathochromic shifts, due to the ICT. The unique photophysical properties of **$[\mathrm{Ir(dfppy)_2(bpy\text{-}Im2)}]^+$** are due to the fast ILET process from ^{3}MLCT(dfppy) to ^{3}MLCT/^{3}LC(bpy-Im2), resulting in the phosphorescence emission originating from ^{3}MLCT/^{3}LC(bpy-Im2). On the other hand, the TA bands of **bpy-Im2** were observed at 540 and 480 nm, corresponding to the singlet and triplet manifolds, respectively. In contrast, the TA spectrum of **$[\mathrm{Ir(dfppy)_2(bpy\text{-}Im2)}]^+$** showed broad bands centered at 420 and 600 nm, attributed to the transitions from ^{3}MLCT(dfppy) and ^{3}MLCT/^{3}LC(bpy-Im2), respectively. Time-resolved spectroscopic results confirm the efficient ILET dynamics from ^{3}MLCT(dfppy) to ^{3}MLCT/^{3}LC(bpy-Im2) in **$[\mathrm{Ir(dfppy)_2(bpy\text{-}Im2)}]^+$**. From the relaxation times determined by SVD analysis and simple sequential kinetic model, we found that the ILET process from ^{3}MLCT(dfppy) to ^{3}MLCT/^{3}LC(bpy-Im2) occurs with a time constant of ~4 ps.

Poster Presentation : **INOR.P-111**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Self-healable rhenium-poly(THF) composite for resilient metal electrode on flexible substrates

Byeong-Yong Jeong, Seok Min Yoon[1,*]

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

The advent of flexible electronics has brought infinite varieties for their powerful penetration into many fields of smart electronics, including artificial e-skin, flexible touch sensors, health monitors, implantable devices, and so on. Metal electrodes such as gold and silver are a crucial component for constructing flexible electronic circuits. However, such metal electrodes spontaneously caused cracking by a mechanical strain diminishing their original electrical conductivity. Nevertheless, surprisingly, developing methods to prevent such cracking have not been unnoticed well compared to advanced new flexible polymer conductors. Here, novel self-healable rhenium (Re)-poly(THF) composite will be introduced, and it is used as a coating layer to prevent cracks of the metal electrodes from retaining their conductivity. Re-poly(THF) composite can be easily polymerized by dissolving Re2O7 in tetrahydrofuran (THF). The Re2O7, as strong Lewis acid, can initiate ring-opening polymerization of the THF. After 48 hours of polymerization, the rhenium-poly(THF) composite was gel-phase, which was analyzed by rheometer. Further, the gel rapidly healed after returning the strain back to 0.5% (for 120 s), which was almost turned back to its initial viscoelastic profile. The Re-poly(THF) composite coated Au electrodes could successfully retain their original electrical conductivity even after 100 times mechanical bending cycles. Further, the electronic circuit coupled with conductive Re-poly(THF) composite could turn on LED bulbs. The lighted LED immediately went off when the circuit was cut off, while the self-healable ability of the Re-poly(THF) composite could recover the electric power supply for turning on the bulb again.

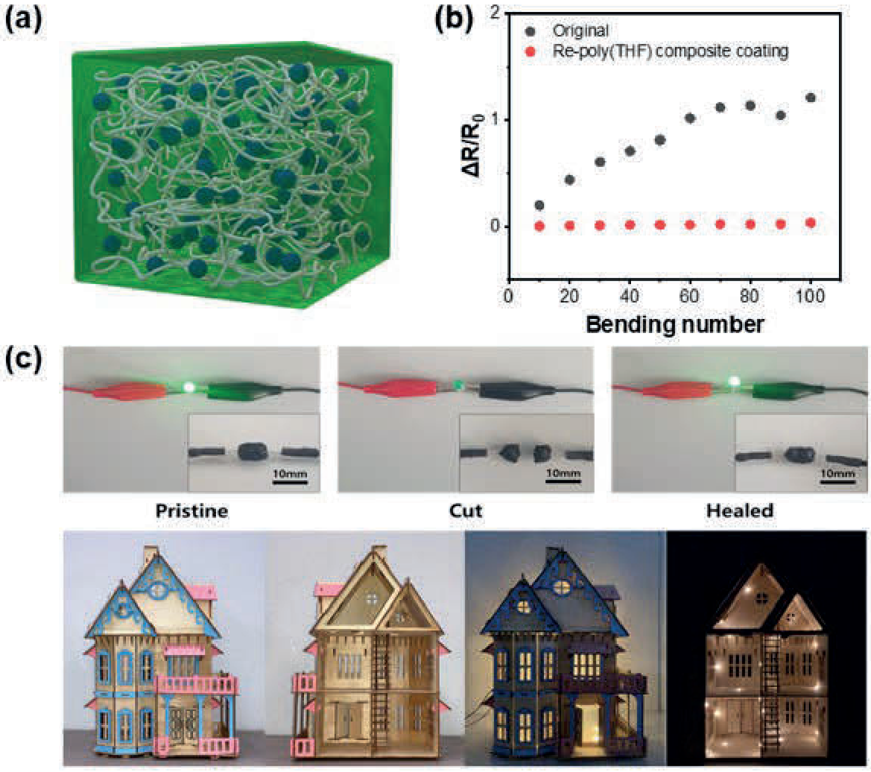


Figure 1. (a) schematic of a rhenium-poly(THF) composite, (b) Resistance change of rhenium-poly(THF) composite on the PET film, (c) Photographs of the rhenium-poly(THF) composite to power an LED.

Poster Presentation : **INOR.P-112**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Photoluminescent characteristics of K2SiF6:Mn4+ phosphors according to the purity of Mn4+ activator

Kangsik Choi, Younbong Park*

Department of Chemistry, Chungnam National University, Korea

A K2SiF6 phosphor using Mn4+ as an activator with narrow emission is very promising for producing white LEDs with excellent luminescence efficiency. In general, the K2SiF6:Mn4+ phosphor is prepared by dissolving KF, SiO2 and K2MnF6 in HF. K2MnF6 is prepared by reducing KMnO4 using H2O2 or oxalic acid. However, the Mn3+ easily appears during the synthesis of KMnF4 and poisons the luminescence efficiency of the final phosphor. Therefore, it is very important to obtain Mn4+ exclusively during the preparation of K2MnF6, which guarantees better luminescence of K2SiF6:Mn4+ phosphor. In this study, single-phase K2MnF6 with Mn4+ were prepared using formic acid instead of the conventional reducing agent. The +4 oxidation state of Mn ion of the final K2SiF6:Mn4+ phosphor prepared was confirmed using XRD and XAS. As a result, single-phase K2MnF6 was synthesized using a new reducing agent, and a K2SiF6:Mn4+ phosphor with better luminescence has been prepared.

Poster Presentation : **INOR.P-113**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Development of ZIF-encapsulated gold nanorod assembly for molecular selective sensing

Suhyeon Park, Juyeong Kim[*]

Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University, Jinju 52828, Korea

We developed a hybrid nanostructure that consists of assembled gold nanorods encapsulated by a zeolitic imidazolate framework-8. We investigated the product formation process by varying reaction time, ligand concentration, and surfactant concentration. Our hybrid material displayed molecular-selective sensing capacity through surface-enhanced Raman scattering. Our synthesis approach will help design innovative hybrid nanomaterials for molecular sensing.

Poster Presentation : **INOR.P-114**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Cellular Senescence Control of 3T3/NIH Fibroblasts Using Replicative Stress and Reactive Oxygen Species

Semin Son, Jin Seok Lee[1,*]

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

Human aging and cellular senescence are known to have a direct correlation. Accordingly, studies to identify the cause of cellular senescence and to overcome it are being actively conducted. Cellular senescence stressors include oncogenes, replicative stress, reactive oxygen stress (ROS), mitochondrial dysfunction, irradiation, and chemotherapeutic drugs. Here in, we have obtained senescent cells with varying degree of aging using replicative stress and ROS. We used mouse-derived fibroblast, 3T3/NIH cells to induce cell senescence by successive passaging (replicative stress) and hydrogen peroxide treatment (ROS). To characterize the degree of aging, we check the cell adhesion area, cell shape, motility change, and beta-galactosidase expression level, which can be indicators of cellular senescence. We will conduct a following experiment to compare the degree of interaction between cells and ECM according to the degree of aging using the senescent cells obtained in this work.

Poster Presentation : **INOR.P-115**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fabrication of Dome-Shaped Porous Alumina Microstructures and Their Applications for Drug Delivery System

Yoobeen Lee, Jin Seok Lee[*]

Department of Chemistry, Hanyang University, Korea

Nano- and micro-sized structures are promising candidates to inject and control of active amount such as drugs or biomaterials into cells. In particular, the porous structures can improve the delivery efficiency in combination with the high surface area. Many previous studies have been investigated drug injection using porous aluminum, carbon nanotubes and nanocapsules as drug delivery systems. However, these drug delivery systems have some limitations in controlling the amount of dugs injected into the cells. Anodization of pre-patterned aluminum substrate can produce highly ordered dome-shaped porous alumina microstructures at desired positions. In this work, we obtained various three-dimensionally dome-shaped porous alumina microstructures array, which are called simply ‘microdome’, by using the imprinting process on the initial surface on a large area with adjustable diameter, thickness, and arrangement. We also investigated the efficiency of microinjection into Hela cells by fluorescence staining experiments to confirm drug delivery into the cells. These platforms can serve as models for novel drug delivery system in many applications.

Poster Presentation : **INOR.P-116**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Investigation on Synergistic Effect of Ag Nanoparticles and Some Extracts to Increase the Efficiency of Dye-Sensitized Photocatalysts

Chaeyoung Moon, Jeong Woo Hong[1], Hee-Jung Im[1,*]

Department of Chemistry & Cosmetics, Jeju National University, Korea
[1]*Department of Chemistry, Jeju National University, Korea*

A photocatalyst is a semiconductor material that generates electrons when it receives light, and one of the most common solar cells using the characteristic is a dye-sensitized solar cell (DSSC). When a dye-sensitized solar cell receives light, it generates electricity through electrons emitted by dye molecules dyed in TiO_2. Compared to silicon-based solar cells, it is inexpensive and can be used while maintaining initial efficiency for a long period of time, attracting attention. However, it has a disadvantage that it is difficult to use in high-output products due to low electrical conversion efficiency. In this study, Ag nanoparticles were used instead of TiO_2 as a dye-sensitized photocatalyst to increase the electrical conversion efficiency of dye-sensitized solar cells, and they were dyed with several plant extracts (such as satsuma mandarin, lemon, and so on). The Ag nanoparticles were characterized by various spectroscopic analyses, and the electrical conversion efficiencies of the two photocatalysts were compared by distinguishing the electrodes coated with TiO_2 and Ag nanoparticles. Electrical conversion efficiency was measured as the change in voltage when exposed to light. In addition, the degree of change in efficiency due to the action of dye and photocatalyst was measured, and the cause was discussed.

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Single-molecule tracking of organic reaction

Minsoo Park

Daegu Gyeongbuk Institute of Science & Technology, Korea

Determining the mechanisms of chemical reactions is a crucial fundamental endeavor. However, Conventional measurements, however, such as UV-vis absorption spectroscopy, mass spectrometer and 1H-NMR can hardly analyze each step of the reaction mechanism and static heterogeneity of kinetics. A single-molecule experiment shows the information hidden in ensembled-averaged methods. Here, to monitor the chemical reaction of individual molecule in real time, we present a reliable method by using organic dyes on total internal reflection fluorescence microscopy (TIRF). TIRF allows us to track the reaction process at single-molecule level due to changes of conjugation length (π-π) and quantum yield. This technique reveals optical properties of each intermediate/transition state in time trajectories which are otherwise difficult to detect with ensemble-averaged measurements.

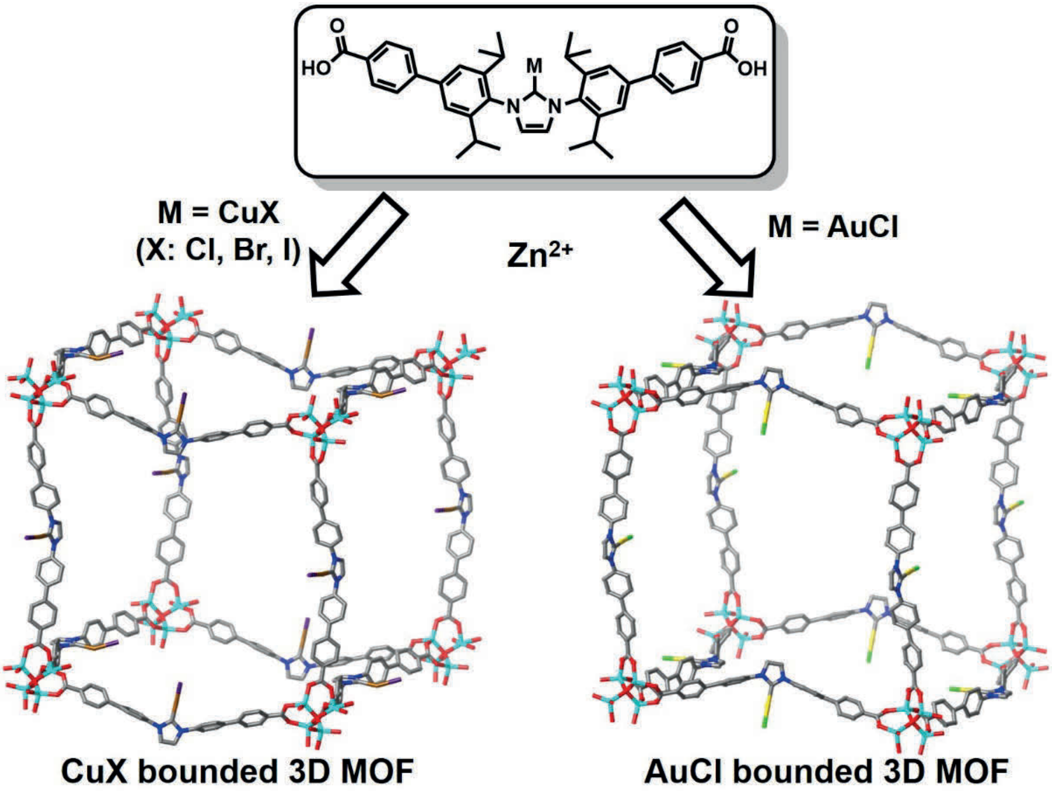
Poster Presentation : **INOR.P-118**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Construction of Stable Metal-Organic Framework Platforms Embedding *N*-Heterocyclic Carbene Metal Complexes for Selective Catalysis

Hyunyong Kim, Eunsung Lee[*]

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

N-Heterocyclic carbene metal complex embedded metal-organic frameworks have been utilized as heterogeneous catalysts. As the bounded catalyst can interfere with framework construction, there are few examples prepared by bottom-up method. Even though these MOFs had well-defined structures, further applications are not demonstrated or there are no size selectivities. Here we report a bottom-up approach to immobilize copper halides and gold chloride into NHC organic linkers in MOFs. Interestingly, the resulting MOFs maintained a 4-fold interpenetrated cube structure. They exhibited high porosity despite the folded structure and high stability in organic solvents, methanol, and water. Moreover, these MOFs exhibited high catalytic activity and size selectivity depending on substrate size in various reactions and can be reused 4 times without significant loss of crystallinity. Incorporation of the various metal complexes into the platform enables the easy preparation of functional MOFs for practical applications.


M
HO
O
N
N
O
OH
M = CuX
(X: Cl, Br, I)
Zn2+
M = AuCl
CuX bounded 3D MOF
AuCl bounded 3D MOF

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Catalytic approach to *in vivo* metabolism of atractylenolide III using biomimetic iron-porphyrin complexes

Hanae Lim, Hyeri Jeon, Hyungbin Park, Seungwoo Hong[*]

Department of Chemistry, Sookmyung Women's University, Korea

Atractylenolide III (AT-III) is a pharmacologically effective phytochemical and is known to be oxygenated during systemic metabolism mainly by cytochrome P450 enzymes (CYP450s), an iron-containing porphyrin-based oxygenase. In the rat plasma samples, the oxygenated metabolite of orally ingested AT-III was determined using liquid chromatography/mass spectrometry and the oxygenated form of AT-III was maintained at higher levels than original form of AT-III. *In situ* catalytic reactions using the iron(IV)-oxo porphyrin π–cation-radical complex, $[(\mathrm{tmp}+\bullet)\mathrm{Fe}^{IV}(\mathrm{O})]^{+}$, demonstrated that both H-atom abstraction and an oxygen rebound mechanism participated in the oxygenation process of AT-III. The density functional theory (DFT) confirmed the oxidative transformation occurred at the 4th and 10th carbon positions of AT-III. Co-treatment with acetaminophen affected differently between *in vivo* and *in situ* models of AT-III metabolism. AT-III was metabolized via oxygenation process in the rat body, where CYP450 and other O_2-activating metalloenzymes might participate in the metabolism. The present work provided the oxidative metabolism of AT-III using *in vivo* model parallel with *in situ* biomimetic reaction models.

Poster Presentation : **INOR.P-120**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Membrane containing Eu-Coordination Polymer Nanoparticles for highly selective detection of phosphate ions

Donggyu Kim, Do Yeob Kim[1], BongJin Jeong[1], Jungseok Heo[2,*], Hyung-Kun Lee[1,*]

화학과, Chungnam National University, Electronics and Telecommunications Research Institute, Korea
[1]*Electronics and Telecommunications Research Institute, Korea*
[2]*Department of Chemistry, Chungnam National University, Korea*

Algae growth has adverse effects on aquatic ecosystems and humans through water pollution. Therefore, a method to detect phosphate, one of the main causes of algal growth, is emerging as an important research area. Monitoring of algae bloom requires many sensors and most of them already have been developed or even commercialized except for phosphate sensors. It has been reported that Eu ions can be utilized for preparation of a sensoring materials through fluorescence quenching in reaction with phosphate. Based on this, luminescent particles in the form of LCPP (luminescent coordination polymer particle) were synthesized through reaction between Eu ions and 2,2'-(5-carboxy-1,3-phenylene)bis(1,3-dioxoisoindoline-5-carboxylic acid) ligands (TCA). LCPP was expected to be an excellent fluorescent probe due to its multiple coordination modes and excellent selectivity against other ions. The synthesized LCPP was embedded in a glass microfiber filter (Eu-TCA/GMF). The limit of detection of Eu-TCA/GMF is 1.52 μM, which is lower than the algae growth indicative level (3.23 μM), confirming that it has excellent detection performances. In addition, it was confirmed that it can be used as a phosphate sensor by showing stability at pH 3 to pH 10 and selectivity to phosphate ions.This work was supported by the ICT R&D program of MSIT/IITP (2018-0-00219, Space-time complex artificial intelligence blue-green algae prediction technology based on direct-readable water quality complex sensor and hyperspectral image).ACKNOWLEDGMENTThis work was supported by the ICT R&D program of MSIT/IITP (2018-0-00219, Space-time complex artificial intelligence blue-green algae prediction technology based on direct-readable water quality complex sensor and hyperspectral image).

Poster Presentation : **INOR.P-121**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Reductive carbonylation of nitroarenes into carbamates using a heterogeneous Pd catalyst

Sudakar Padmanaban, Sungho Yoon[1,*], Yunho Lee[2,*]

Department of chemistry, Seoul National University, Korea
[1]*Department of Chemistry, Chung-Ang University, Korea*
[2]*Department of Chemistry, Seoul National University, Korea*

The reductive carbonylation of nitroarenes in presence of alcohol and CO(g) is one of the interesting alternative routes, which avoids the use of toxic phosgene and corrosive HCl generation, for the synthesis of industrially useful carbamate compounds that serve as the important intermediates for the polyurethane production. Palladium catalysts supported by phen (phen = 1,10-phenanthroline) are known to be effective for this catalysis. In this study, we report the synthesis of a phen-based heterogeneous Pd catalyst, Pd@phen-POP, which involves the solvent knitting of a phen scaffold via the Lewis-acid-catalyzed Friedel–Crafts reaction using dichloromethane as a source for linker in the presence of $AlCl_3$ as a catalyst. The resulting solid material was thoroughly characterized by various physical methods and reveal high porosity and surface area. As similar to the homogeneous pallidum catalyst, this heterogeneous catalyst reveals efficient reductive carbonylation of various nitroarenes. The catalytic reaction using nitrobenzene as a model compound, presents a high turnover number (TON = 530) and a reasonable turnover frequency (TOF = 45 h–1), with high selectivity (92%) for the carbamate formation during the reductive carbonylation of nitrobenzene. According to the recycling studies, the heterogeneous catalyst Pd@phen-POP is recyclable and retains ~90% of the original reactivity in each cycle.

Poster Presentation : **INOR.P-122**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Evaluation of Through-Space Electronic Coupling in the Cofacially Aligned π-Stacked Organic Mixed-Valence System

Eunji Im, Youn Kyung Kang*

Department of Chemistry, Sangmyung University, Korea

Electronic interactions between redox active units that are not directly connected by chemical bonds, which are called through-space interactions compared to its through-bond counterpart, have been of great interest in the electron transfer community. While there have been reported a number of representative structural motifs for through-space electronic interactions that include cyclophanes, 1,2-phenylene derivatives, and bicycloalkanes, here we report a newly synthesized 1,8-bis(2',5'-dimethoxy-4'-methyl-[1,1'-biphenyl]-4-yl)naphthalene (1) as a precursor molecule for a organic mixed-valence system. Structural geometries of neutral, monocationic and dicationic version of 1 were obtained via using density functional theory (DFT) calculations with a range-separated hybrid functional and dispersion corrections (LC-wPBE-D3). Two dimethoxytoluene redox centers were aligned in parallel with van der Waals interplanar distances (3.50–3.70 Å). The electronic coupling (H_{12}) in this Mixed-Valnece System was evaluated by two different approaches : (1)Mulliken–Hush analysis of intervalence charge transfer (IVCT) band obtained from the spectroelectrochemical method usinag an OTTLE cell, and (2) partial charge distribution analysis of quinonoidal distortion of $D^{\bullet+}$ /D centers obtained from theoretical DFT calculations. The H_{12} values were 2055 and 1903 cm^{-1} by (1) and (2), respectively. These results suggest that a pure through-space electronic coupling between two aromatic redox centers, which are cofacially aligned in a parallel manner in the weak van der Waals range and not necessarily be in the perfectly eclipsed position, can be substantial even without a significant compression.

Poster Presentation : **INOR.P-123**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Guest Responsive Reversible Structural Flexibility and Selective Adsorption of C_8 Alkyl Aromatics in Zn-Based Metal-Organic Frameworks

Purna Chandra Rao, Prabu Mani, Younghu Son[1], Minyoung Yoon[*]

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

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

Metal-organic frameworks (MOFs) are a class of crystalline porous materials, comprising metal ions and organic linkers connected through coordination bonds and having numerous structural networks in 1D, 2D and 3D directions. The structural flexibility of MOFs through breathing phenomena has gained significant interest in gas and chemical separation, and sensing technologies. In breathing MOFs, the structural phase transitions are highly dependent on the chemical nature and host-guest interactions with framework networks. In addition, these specific interactions that enable the selective adsorption and separation of several industrially valued-products. Among them, purification of C_8 alkyl aromatics such as o-xylene, p-xylene, m-xylene and ethylbenzene still remains challenges owing to their similar molecular structures, boiling points, kinetic diameters, polarities, etc. With this attention, we have synthesized two isostructural pillar-bilayered Zn-based MOF compounds; denoted as $[Zn_2(aip)_2(pillar)]$; aip = 5-aminoisophthalic acid; pillar: bpy = 4,4'-bipyridine or bpe = 1,2-bis(4-pyridyl)ethane. The structure analysis and compounds properties such as phase purity, thermal stability, and porosity were characterized through various instrumental analyses. The guest sorption studies of both MOFs for various organic solvents such as N,N-dimethylformamide (DMF), methanol, benzene, and water vapour exhibited reversible structural flexibility through breathing phenomena and proposed the guest dependent structural transformation. Interestingly, the obtained activated crystal structural analysis (guest DMF removed framework) of both compounds have demonstrated the attributed reasons for structural flexibilities. In addition, the exciting sorption results provoked us to study the breathing effect and performance of structural changes using C_8 alkyl aromatics in both MOF compounds. As excepted, the both compounds can open the pores and closed the pores upon inclusion and exclusion of these isomers vice versa. These Zn-MOFs exhibit selective adsorption properties

in C_8 binary mixtures based on their associated interactions between C_8 guest aromatics and framework structures. For the demonstration of practical application of the material in C_8 isomer separation, breakthrough experiments for selected C_8 isomer will be also presented.

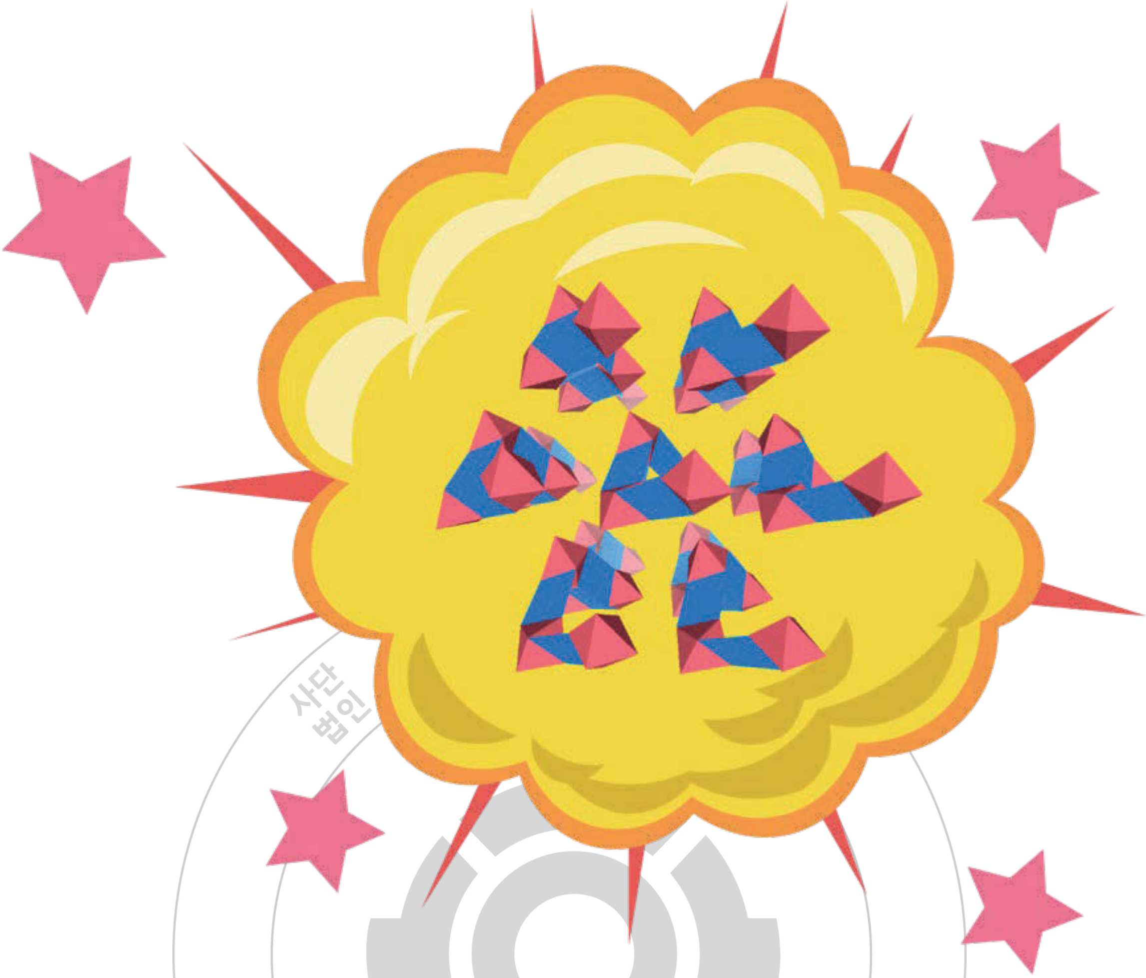
Poster Presentation : **INOR.P-124**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Metal-Organic Nanowires for Energetic Application

Hyeonsoo Cho, Yeongjin Kim, Soochan Lee, Kuktae Kwon[1], Hae-Wook Yoo[1,*], Hoi Ri Moon[*], Wonyoung Choe[*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1] *Agency for Defense Development, Korea*

Energetic materials are used widely in modern society, ranging from civil and military to aerospace industry. These energetic materials store energies inside molecules and detonate from external stimuli, and are still being developed for safety through several changing factors. We synthesize the metal-organic nanowires (MONs) using 5,5′-bistetrazole-1,1′-diol (BTO) linker, N,N-dimethylacetamide (DMA) solvent, and together with Cu and Mn metal cations. The new crystals, MON-1 and -2, show different 1D structures, straight and helical types. The comprehensive studies of structures, energetic properties, and sensitivity are conducted, and these two compounds showed excellent thermal stability. The detonation properties of MON-2 are comparable to previously published BTO-based energetic materials. These MONs reveal excellent insensitivity due to the long wire-to-wire distance originated from DMA solvents. Therefore, the solvent molecule should be regarded as a component and affects the detonation properties and sensitivity of the energetic materials together with metal and linker.



Poster Presentation : **INOR.P-125**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

New Aluminum-based catalysts for CO_2 conversion

Soeun Ha, Jimin Jeon, Youngjo Kim*, Myung Hwan Park[1,*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemical Education, Chungbuk Natioanl University, Korea*

The cycloaddition of CO_2 to epoxides yielding cyclic carbonates, used as aprotic polar solvents, electrolytes for lithium–ion batteries, monomers for polymerizations, and pharmaceutical intermediates, is one of the most important consumption and/or transformation methods of CO_2 as a C1 feedstock due to the atom economy principle (no side products) and the broad applicability. Several catalyst systems, including metal-based catalysts and organocatalysts, have been reported for converting CO_2 into cyclic carbonates at room temperature and 1 bar CO_2. Aluminum, the most abundant metal in the earth's crust (the metals are in the order Al, Fe, Ca, Na, K, Mg, and Ti), is a particularly attractive metal for this study, owing to its low cost, low toxicity, and high Lewis acidity. However, only a few examples of efficient nontoxic catalysts with aluminum metal centers capable of operating at ambient temperature and 1 bar CO_2 are known. In this poster, we will present the synthesis and characterization of new aluminum-based complexes, and their catalytic activities for the coupling reaction of CO_2 and epoxides under the condition of atmospheric CO_2 pressure and ambient temperature.

Poster Presentation : **INOR.P-126**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Metal Complex Bearing Bidentate Cyclic (Alkyl)(Amino)Carbenes (cAACs)

Jang Minjae, Dae Young Bae[1], Hayoung Song[1], Eunsung Lee[1,*]

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

Cyclic (alkyl)(amino)carbenes (cAACs) have drawn great attention because of their more outstanding amphiphilic ability than N-heterocyclic carbenes (NHCs). Because of this, cAACs could stabilize low valent metal complexes or organic radicals, and Bertrand-Grubbs catalyst could show remarkable restriction of isomerization. Unlike NHCs, only recently synthesis of bidentate cAACs was reported by the Bertrand group due to synthetic difficulties. Nevertheless, the application of these bidentate cAACs remains rare. Herein, we report the new metal complex bearing bidentate cAACs. The metal complex was characterized by NMR spectroscopy and single-crystal X-ray diffraction analysis. Examination of the reactivity of this metal complex is now in progress.

Poster Presentation : **INOR.P-127**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Efficient Synthesis of Block, Gradient, and Random Copolymers via Ring-Opening Copolymerization of Caprolactone and Lactide Using Aluminum Catalyst

Yoseph Kim, Yeonsoo Kim, Myung Hwan Park[1,*], Youngjo Kim[*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemical Education, Chungbuk Natioanl University, Korea*

Random copolymers derived from lactide (LA) and caprolactone (CL) have great potential in a wide range of application areas. It is generally known that the homopolymerization of CL is faster than the homopolymerization of LA, but the consumption rate of CL in copolymerization is much slower than that of LA. (rCL << rLA). Thus, the synthesis of truly random copolymers is very challenging. In addition, the subtle modified microstructure of copolymers such as poly(LA-grad-CL) or block, poly(LA-block-CL) is extremely difficult project. Until now, the synthesis of block, gradient, and random copolymers for LA and CL using single catalytic components have not been reported in the literature. The detailed synthesis, characterization, and catalytic activity of new aluminum compounds will be discussed.

Poster Presentation : **INOR.P-128**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Highly Selective Sensing for Heavy Metal Ion by a NS_4-Macrocyclic Chemosensor

Yelim Lee, Joon Rae Kim, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

Synthesis and sensing properties of macrocyclic chemosensor showing highly selectivity for toxic heavy metal ions such as mercury(II), lead(II), and cadmium(II) are reported. The benzothiazolyl group bearing NS_4-macrocycle (**L**) as a chromoionophore was synthesized by the reaction of N-phenylaldehyde macrocycle with 2-aminobenzenethiol. The macrocyclic chemosensor **L** showed mercury(II) selectivity over other metal ions by UV-vis and fluorescence spectroscopy in acetonitrile. Now, the complexation studies of structure−function relationship for the anion dependency on the mercury(II) sensing is in progress.

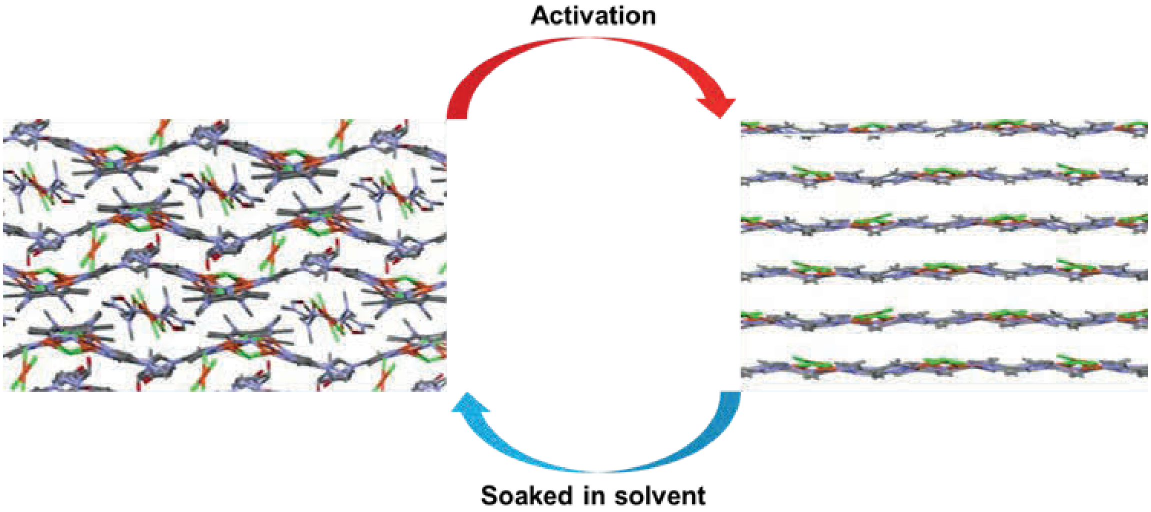
Poster Presentation : **INOR.P-129**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Flexible Cu(I)-2D MOF: Solvent dependent single crystal to single crystal (SC-SC) conformation change

Younggyu Seo, Eunsung Lee*

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

Metal-organic frameworks (MOFs) are composed of metal nodes and organic linkers. MOFs have permanent porosity and are used for various applications such as gas separation, gas storage, catalysis, chemical sensing, and so on. MOFs have different dimension structures, 0D-to-3D. Moreover, some of MOFs have flexibility in structural change, we called that MOFs are flexible-MOFs.2D-MOFs are one type of flexible-MOFs. Flexible-MOFs are also called soft-porous crystals (SPCs). SPCs are changed their structures due to external stimuli such as solvent exchange, solvent removal, heat, light-response, or pressure. Using this property, we can control the pore size and used it for various applications, gas storage, separation, catalysis, and so on. Here, we report the flexible Cu(I)-2D MOF, which exhibit the solvent dependent single crystal-to-single crystal (SC-SC) conformation change. Cu(I)-2D MOF shows reversible conformation change which can be easily exchanged to different solvent without any structural decomposition. With this property, we could expect to be able to utilize Cu(I)-2D MOF in various applications such as catalysis, conductivity, or photo reductions.


Activation
Soaked in solvent

Poster Presentation : **INOR.P-130**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Mixed Copper States of Anion-doped Cu_3N Nanocubes for Improved C_{2+} Selectivity in CO_2 Reduction Reaction

Duck Hyun Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Recently, closing the carbon cycle by converting carbon dioxide into usable fuels and chemical reagents is on the issue of many researchers, and C_{2+} products are gaining significant attention for their numerous applicability in various fields. Among a number of catalysts, Cu-based nanocatalysts show outstanding performance for C_{2+} selectivity in electroreduction of CO_2 due to the ensemble effect of Cu^0 and Cu^+, and Cu_3N nanocubes successfully stabilize Cu^+ during the electroreduction. Herein, we synthesized sulfur- and phosphine-doped Cu_3N nanocubes as electrocatalysts for the CO_2 reduction reaction. The prepared multi-anion copper compound catalysts are expected to exhibit improved selectivity of C_{2+} products compared to pristine Cu_3N catalysts.

Poster Presentation : **INOR.P-131**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Pt-Embedded Ruthenium Phosphosulfide Nanotubes as Enhanced Electrocatalysts toward the Hydrogen Evolution Reaction in Alkaline Media

Soo Bean Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

The concern of environmental pollution and diminishing fossil fuels has been accelerated the research on eco-friendly energy. In view of this, hydrogen production through hydrogen evolution reaction (HER) has been reported as a promising strategy due to its eco-friendly process. Since synergistic effects between nano-scale materials can enhance the alkaline HER performances, heterostructure catalysts have been reported during the past few decades. However, the heterostructures have the disadvantage that is limiting active surface area for HER. Herein, we synthesized platinum-ruthenium phosphosulfide nanotubes ($(PtRu)P_{2-x}S_x$ NTs) by partial cation exchange reactions. The alternating platinum and ruthenium can play critical roles in alkaline water dissociation and hydrogen productions, respectively. We expect that the localization of distinct active sites in phosphorus anion frameworks can maximize the synergistic effect between platinum and ruthenium. Furthermore, to maximize the surface area, we fabricated the morphology of the electrocatalyst into double-walled nanotubes. Due to this unique strategy, our double-walled ruthenium phosphosulfide nanotubes (DW-$(PtRu)P_{2-x}S_x$ NTs) exhibit outstanding performance.

Poster Presentation : **INOR.P-132**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Ternary Intermetallic Nanoframe as Oxygen Reduction Electrocatalyst

YunChang Son, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

A fuel cell has been received enormous attention as one of the most promising energy conversion systems; however, being suffered from sluggish kinetics of the oxygen reduction reaction (ORR). Although Pt-based binary catalysts show excellent initial activities, their low durability caused by the dissolution of non-Pt elements during electrocatalysis poses a great challenge for the practical application in fuel cell devices. Meanwhile, Pt-based ternary alloy or intermetallic alloy materials exhibit strong orbital interactions between different metal atoms, which results in higher phase stability and thus suppressed dissolution under harsh electrocatalytic conditions. Herein, we report the synthetic strategy of Pt-based ternary ordered nanocatalysts via protective layer assisted-method, which prevents the morphological deformation of the hollow structure during the thermal annealing process. Pt-based ternary intermetallic nanoframes might exhibit enhanced ORR activity and durability due to their high surface area and improved phase stability, respectively.

Poster Presentation : **INOR.P-133**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Introducing Heteroatom into Cu_2O Nanocatalysts for Enhancing the NH_3 Selectivity during Electrochemical Nitrate Reduction

Hyoryung Choi, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Ammonia (NH_3) plays a vital role as a green energy carrier and feedstock in the chemical industry. Lately, aqueous-based electrosynthesis of NH_3 from NO_3^- reduction reaction (NO_3RR) has been regarded as an alternative approach for NH_3 production because of its environment-friendly and sustainable strategies. However, the sluggish kinetics of NO_3RR is a hurdle that should be overcome. Therefore, it is highly desirable to design the electrocatalysts for improving the adsorption of NO_3^- and enhancing the formation of NH_3, suppressing the hydrogen evolution which is a competitive reaction. In this work, we synthesized the heteroatom-Cu_2O nanocomposites, resulting in the modulation of adsorption energy for intermediates. Notably, palladium has the ability to adsorb hydrogen, which can facilitate the formation of N-H bond, thus, Pd-Cu_2O nanocatalysts might exhibit superior catalytic performance, compared to the only Cu_2O nanocrystals and commercial Pd catalyst.

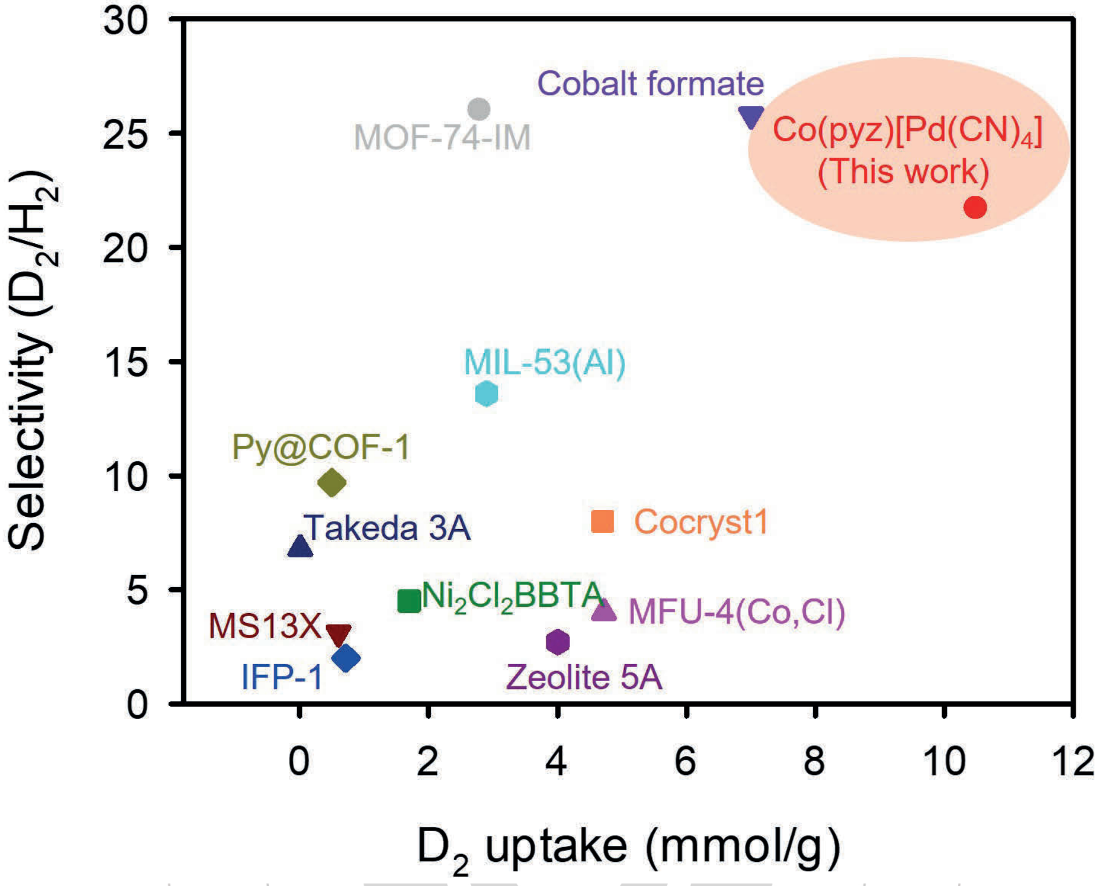
Poster Presentation : **INOR.P-134**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synergistic Quantum Sieving Effects in Hofmann-type Metal-Organic Frameworks for Hydrogen Isotope Separation

Junsu Ha, Hyunchul Oh[1,*], Hoi Ri Moon[*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Energy Engineering, Gyeongnam National University of Science and Techn, Korea*

Hydrogen isotopes, especially deuterium possesses critical role in various scientific area, e.g., biomedical applications, nuclear fusion, energy resource, and so on. Despite the high demand, hydrogen isotope separation is very challenging because of the identical physicochemical properties between the isotopes and extremely low natural abundance (0.0156 %) of deuterium. Conventional deuterium production methods such as cryogenic distillation and Girdler sulfide process only provide low separation factor (~ 2.5) with large energy consumption. Herein, we prepared a Hofmman-type MOF, $Co(pyz)[Pd(CN)_4]$ for highly efficient isotope separation, which shows high separation factor of 21.7 as well as high D2 uptake of 10.5 mmol/g at 25 K. This is attributed to the synergistic effect of high density of Pd^{2+} open metal sites (OMSs) and a narrow pore aperture (3.6 Å) in $Co(pyz)[Pd(CN)_4]$, which is responsible for chemical affinity quantum sieving (CAQS) and kinetic quantum sieving (KQS) effects, respectively.



30
25
20
15
10
5
0
Selectivity (D_2/H_2)
0
2
4
6
8
10
12
D_2 uptake (mmol/g)
Cobalt formate
MOF-74-IM
Co(pyz)[Pd(CN)$_4$]
(This work)
MIL-53(Al)
Py@COF-1
Takeda 3A
Cocryst1
Ni_2Cl_2BBTA
MFU-4(Co,Cl)
MS13X
IFP-1
Zeolite 5A

Poster Presentation : **INOR.P-135**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fluorescence Detection of Glutathione Using Au(I) Bis(*N*-heterocyclocarbene) Complex

Shinae Lee, Seunga Heo[1], Youngmin You[2,*]

Chemical Engineering & Materials Science, Ewha Womans University, Korea
[1]*Ewha Womans University, Korea*
[2]*Chemical Engineering and Materials Science, Ewha Womans University, Korea*

Biothiols constitute peptides and play important roles in a variety of pathophysiological processes in the human body. In particular, glutathione (GSH) plays critical roles in immune systems, cancer prevention, detoxification, and anti-aging. In order to maintain these functions, intracellular levels of GSH are tightly regulated. Failures of the GSH homeostasis is conceived to result in fatal pathological conditions. It is, therefore, of central importance to monitor GSH with high precisions. However, conventional techniques are not suitable for monitoring GSH because they are invasive and require pretreatments of samples. We discovered that an Au(I) complex having two 1,3-diphenyl-1H-benzo[*d*]imidazole-3-ylidene (BZI) ligands (i.e., $[Au(BZI)_2]^+$) can fluorescently visualize GSH. $[Au(BZI)_2]^+$ was prepared through the dechlorinative ligand scrambling reaction of [Au(BZI)Cl] in the presence of silver(I) perchlorate in CH_3CN. The chemical structure of $[Au(BZI)_2]^+$ was analyzed by ^1H NMR spectroscopy and ESI-MS analyses. $[Au(BZI)_2]^+$ displays weak blue emission (λ_{em} = 442 nm) in a buffered aqueous solution (pH 7.4) containing 25 mM piperazine-*N,N′*-bis(2-ethanesulfonic acid) (PIPES), 100 mM KCl, and 64 vol % DMSO. The addition of GSH elicits a fluorescence signaling with a 4-fold increase in the fluorescence intensity and a red shift in the fluorescence peak wavelength (λ_{em} = 478 nm). The fluorescence response is selective to GSH over other biological Lewis bases, including amino acids, small molecular neurotransmitters, metabolites, and nucleosides.

Poster Presentation : **INOR.P-136**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Electornically tunable cyclic(alkyl)(amino) carbene system: Indol-2-ylidene

Hyunho Kim, Minseop Kim[1], Hayoung Song[*], Eunsung Lee[*]

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

N-heterocyclic Carbenes (NHCs) have regarded as useful tool in chemistry. Because of their unique electronic properties, NHC show interesting reactivity and various abilities. In 2005, Guy Bertrand group developed new class of NHC, Cyclic (alkyl)(amino) Carbenes (CAACs) which enhance ambiphilic properties. By replacing one nitrogen atom to alkyl group, CAACs have more electrophilic properties, while retaining the nucleophilic character. Thanks to the ambiphilicity, CAAC ligands have been applied in diverse fields such as light-emitting materials as CAAC-Cu complexes and novel transition metal catalysis.Based on CAACs, other classes of ambiphilic NHCs have been developed, Cyclic (amino)(aryl) Carbenes (CAArCs). The ambiphilicity of CAArCs could be increased by introducing aryl group to CAAC platform. In the same vein, the indole scaffold is a promising candidate for ambiphilic NHCs due to its cyclic (alkyl)(amino) fragment and the presence of an aryl group, in close resemblance to known ambiphilic NHCs.Herein, new class of NHC ligand was synthesized, indol-2-ylidene (IdY), which is derived from indole scaffold. Indolenium precursor could be prepared on a gram scale with good yields. Trapping experiments with selenium, [RhCl(cod)]2 and CuCl afford carbene adducts. Computational and experimental data supported the ambiphilicity of IdY, which lies between CAACs and CAArCs. The copper adduct complex show high percent buried volume (% Vbur = 58.1) and allow for carboboration of terminal alkynes within 30 minutes.

Poster Presentation : **INOR.P-137**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Proton conductivity on MOF using sulfonate groups

Seungjae Park, Eunsung Lee*

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

Metal-organic frameworks (MOFs) are representative robust and porous crystalline materials consisting of metals and organic linkers. In the past few decades, numerous metal-organic frameworks (MOFs) and their synthetic methods have been reported to develop their interesting applications tuning their clusters and linkers. Typically, the gas separation, catalysis, and conductivity are investigated for their applications. In this study, proton conductive material was synthesized with rigid structure and high conductivity. The material was synthesized by zinc and monosodium 2-sulfoterephthalate as the linker. Two different structures were obtained in different synthetic conditions. It was characterized by the powder X-ray diffraction, gas adsorption, and conductivity on various temperature and relative humidity.

Poster Presentation : **INOR.P-138**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mercury(II)-Selective and Anion-Controlled Macrocyclic Chemosensor

Joon Rae Kim, Yelim Lee, Eunji Lee*

Department of Chemistry, Gangneung-Wonju National University, Korea

Chemosensor exhibiting high selectivity for toxic heavy metal ions have been of widespread interest due to the environmental importance such as bioaccumulation. The benzothiazole-attached macrocyclic chemosensor (**L**) with a NO_2S_2 donor set as a dual-probe channel (UV−vis and fluorescence) chemosensor was synthesized. **L** showed fluorescence turn-off type mercury(II) selectivity with ClO_4^- and NO_3^-. However, the addition of mercury(II) salts with the other anions (Cl^-, Br^-, I^-, SCN^-, and $CF_3CO_2^-$) showed no spectral change. The detailed complexation process with mercury(II) perchlorate associated with the cation sensing was also monitored with the titration methods by UV-vis, fluorescence spectroscopy.

Poster Presentation : **INOR.P-139**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Triple C–F Bond Activation of Fluoroarenes by N-heterocyclic Carbenes Generating Trisubstituted N-Heterocyclic Imidazoliums

Seoung Su Kim, Eunsung Lee[1,*]

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

N-heterocyclic carbenes (NHCs) has been considered as major candidate for activating and stabilizing small molecules directly with its strong sigma-donability and pi-acceptability, which was the domain of reactivity of transition metal chemistry. We have been exploring activation of C–F bonds, the strongest single bond in organic chemistry, utilizing NHCs for various applications such as catalysis and material science. Reacting octafluorotoluene of IPr (well-known NHCs), unexpected sequential substitution of fluorides in two separate rings to afford tetrasubstituted imidazolium salt, is one successful result we previously reported. Here we tried better and challenging extension, the triple C–F bond activation of fluoroarenes by N-heterocyclic carbenes (IMes and IPr) generating trisubstituted N-heterocyclic imidazoliums as a new redox materials. The synthesis and properties of the novel compounds will be discussed.

Poster Presentation : **INOR.P-140**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Stille Coupling-based Hollow Conjugated Microporous Photocatalysts for Visible Light-Induced Hydrogen Evolution

Seung Uk Son[*], Sang Hyun Ryu

Department of Chemistry, Sungkyunkwan University, Korea

Recently, there have been great studies of scientists on conjugated microporous polymer (CMP)-based organic photocatalysts for hydrogen evolution, showing gradually improvement of the hydrogen evolution rates (HERs) from 70 μmol h^{-1} g^{-1} to 3106 μmol h^{-1} g^{-1}. The HER performance of CMP-based photocatalysts is epxpected to be dependent on their morpholgies. In the materials chemistry, it has been reported that the hollow structural engineering of catalysts can enhance their performance. However, as far as we are aware, there have been no reports on the hollow CMP-based photocatalysts, due to the limited synthetic methods. This work shows that HER performance of CMP-based photocatalysts can be dramatically enhanced through hollow shape engineering. Using a hollow microporous organic polymer (H-MOP) as a template, hollow Stille coupling-based CMP photocatalysts could be synthesized. Interestingly, because the Stille coupling reactions required zerovalent Pd catalysts without additional bases, the Pd nanoparticles could be concomitantly engineered into the hollow catalysts. The resultant H-MOP@SCMP-Pds showed the promising HERs up to 7100 μmol h^{-1} g^{-1} and apparent quantum yields up to 3.72% (420 nm). Interestingly, in the synthetic strategy of this work, while the H-MOP platform induced the hollow shape engineering of H-MOP@SCMP-Pds, at the same time, it faciltated the neworking reactions in the formation of SCMP to result in the enhanced surface area and microporosity. The HER performance of the optimized H-MOP@SCMP-Pd2 is superior to the recent CMP-based photocatalysts with Pd species. The excellent HER performance of H-MOP@SCMP-Pd2 can be attributable to the harmonized amount of SCMP and Pd nanoparticles, the high surface area and porosity, and the hollow structure-induced short diffusion pathways of redox substrates.

Poster Presentation : **INOR.P-141**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Defective CeO_2 in a hollow carbon matrix as a hydroxide-assisted high performance pseudocapacitive material

Hyeonseok Jeong, Seung Uk Son[*]

Department of Chemistry, Sungkyunkwan University, Korea

CeO_2 is an intriguing material. When the size of CeO_2 materials is reduced to nanoscales, the oxygen vacancies and the resultant Ce^{3+} species are enhanced. Because the Ce^{3+} is redox active, the nanoparticulate CeO_2 can be a promising pseudocapactive material. To be utilized as pseudocapacitive energy storage materials, the size control of CeO_2 to nanoregimes is important. In addition, the defective CeO_2 can be incorporated into a conductive carbon matrix to improve its conductivity. However, the systematic shape engineering of CeO_{2-x} based composite materials has been relatively less studied. This work showed that microporous organic polymer (MOP) chemsitry can be applied to the engineering of nanoparticulate CeO_2 in a carbon matrix. Hollow MOP platforms could be utilized for the engineering of the nanoparticulate CeO_2 in a hollow carbon matrix (H-C@CeO_2). The H-C@CeO_2 showed high specific capacitances up to 527(@0.5 A/g), 493(@1 A/g), and 458 F/g(@10 A/g) in alkaline electrolyte. In addition, the H-C@CeO_2 showed excellent cycling performance for 10000 cycles. We suggest that the hydroxide ions facilitate the redox behavior of the defective CeO_2 through the coordination to the oxidized Ce species. The electrochemical performance of H-C@CeO_2 in this work is superior to the CeO_2-based pseudocapacitive materials in the literature including the nano-engineered CeO_2, the doped CeO_2, and CeO_2-carbon composites. The promising electrochemical performance of H-C@CeO_2 is attributable to the hollow structure, the nanoparticulate CeO_2 with the Ce^{3+} species, and the enhanced conductivities by the carbon matrix.

Poster Presentation : **INOR.P-142**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Revisited reaction-path simulation of the paddle-wheel-like complex formation of tetrakisacetatodimolybdenum(II) from monomers

Hyo Weon Jang

Department of Chemistry, Suncheon National University, Korea

We propose another results for the previously studied reaction path for the title-mentioned reaction. The main difference is centered on the earlier part where two intact octahedral monomer units are joined by van der Waals forces to form a dimer posing as a dual-cube sharing a common edge. Successive eliminations of acetic acid ligands followed by forming acetato-metal bridges between monomers produce various dimer complexes containing various 8, 7 and 6-coordination ligand-metal. Final step involves metal-metal bond formation and expulsion of last acetic acid ligands producing the final form of dimer. The overall path is expected to be thermally accessible judging from the calculated activation energy barriers.

Poster Presentation : **INOR.P-143**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Room Temperature Synthesis of Hollow Microporous Organic Polymer Bearing Activated Alkynes as IR probes for Post-Functionalization

June Young Jang, Seung Uk Son[1,*]

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

Microporous organic polymers (MOPs) can be prepared by Sonogashira-Hagihara coupling. Weber et al. reported the post-synthetic modification (PSM) of MOPs based on the radical-induced thiol-yne click chemistry. Since then, various functional MOPs have been prepared by the post-synthetic modification (PSM) based on the thiol-yne click reaction. However, the conventional PSM of MOPs by the radical-induced thiol-yne reaction has three weak points. First, according to our previous studies, thiols are added to the defect sites of MOPs. Compared to facile molecular click chemistry, the reactivity of internal alkynes in the main chain networks of MOPs are suppressed by a network-induced constraint. In the solid state ^{13}C NMR spectroscopy, most internal alkynes in the main chain networks of MOPs were actually intact in the radical-induced thiol-yne click reaction. Thus, we suggest that more exploration is required for MOP bearing activated alkynes. Second, the radical-induced thiol-yne reaction is powerful in the incorporation of thiols to alkynes. In comparison, nonradical thiol addition to internal alkynes is relatively less efficient. In addition, thiols with radical quenching moieties can be inefficient in the radical-induced thiol-yne reaction. If the reactivities of internal alkynes can be enhanced, thiols can be added without the help of radical species. Third, the monitoring of the PSM of MOP is important and challenging. The IR spectroscopy is a convenient tool. However, the IR vibration peaks of internal alkynes in the conventional MOP are very weak in intensity. Thus, the IR monitoring of thiol-yne-based PSM of MOP is inefficient. This work introduces the template synthesis of hollow MOP-A by acyl Sonogashira coupling. The H-MOP-A has four benefits. First, the H-MOP-A could be prepared at room temperature. Second, the H-MOP-A has activated alkynes and can be functionalized by non-radical thiol addition. Third, the IR peaks of alkynes in H-MOP-A were very sharp and strong in intensity, due to the asymmetric chemical surroundings. The alkynes in H-MOP-A can act as an IR probe of the PSM. Finally, this work shows the applications of post-functionalized H-MOP-A. The functionalized hollow H-MOP-CA-Ag showed excellent catalytic

performance in the room temperature CO_2 fixation with propargyl alcohols to α-alkylidene cyclic carbonates, due to the well-distributed anchoring groups and Ag^+ ions.

Poster Presentation : **INOR.P-144**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Pb-free highly stable and blue emitting perovskite film

Hyeongjin Lee, Sang Wook Park[1], Young rag Do[2,*]

Department of Applied Chemistry, Kookmin University, Korea
[1]*Department of Chemistry, Kookmin University, Korea*
[2]*Department of Bionano Chemistry, Kookmin University, Korea*

Perovskite has been studied a lot in the field of light emission because of its low production cost, easy synthesis, and good optical property. Currently, among various types of perovskite, lead-based perovskite is the most efficient and has good optical properties. However, because Pb is harmful for human health and the environment, a lot of research has been done on perovskite that does not contain Pb. However, perovskite without Pb was found to have low efficiency, or the emission wavelength was not suitable for use as RGB. In this work, we synthesized Pb-free Cu-based blue emitting perovskite. The photoluminescent quantum yield (PLQY) is high (87.3%) and the emission peak wavelength is blue (448nm). Even compared to conventional lead-based perovskite ($CsPbBr_3$), this material has excellent thermal stability, polar solvent stability, and UV stability. This material was deposited as a film and the film also had very high PLQY and stability. It was confirmed through XPS that Cu has a monovalent oxidation state; stoichiometry and crystal structure of $Cs_3Cu_2I_5$ were confirmed through EDS and XRD. This material can be used in various lighting applications such as LEDs and phosphors.

Poster Presentation : **INOR.P-145**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Selective Synthesis of Iridium and Ruthenium Supramolecules Using Various Tetrazolyl Lignads

Jeonghyeon Park, Junseong Lee[*]

Department of Chemistry, Chonnam National University, Korea

It is still remained as a big challenge to modulate the structures of supramolecular architectures in spite of tremendous researches on supramolecular chemistry. The coordination-driven self-assembly of metal ions with electron donating groups such as pyridine has been considered as one of most convenient methods. However, the assembly is reversible and researches have tried to use more strong interactions for the formation of concrete supramolecules. Ru complexes containing tetrazolyl ligands have been extensively studied and there are several interesting reports on the synthesis of half-sandwich Ru complexes containing one, two, or three bridging tetrazolyl ligands. Herein, we report the formation of multinuclear ruthenium and iridium supramolecular complexes via the bridge-driven self-assembly of tetrazolyl ligands. The synthesis of dimeric half-sandwich Ru units was made by the reaction of half-sandwich Ir and Ru units and tetrazolyl ligands in a molar ratio of 1:2. The bridging modes of tetrazolyl ligands influence to the architectures of Ir and Ru supramolecules such as rectangular, truncated trigonal pyramidal and truncated tetrahedral structure. The rectangular structure was obtained from the reaction of 1,2-ditetrazolyl benzene, [(p-cymene)2RuCl2]2, AgOTf in molar ratio of 1:1:3. From 1,2-, 1,3-ditetrazolyl benzene and 1,3,5-tritetrazolyl benzene, new Ir and Ru supramolecules were synthesized via bridge-driven self-assembly and characterized by IR, 1H, 13C NMR spectroscopy, and Electrospray ionization mass spectrometry.

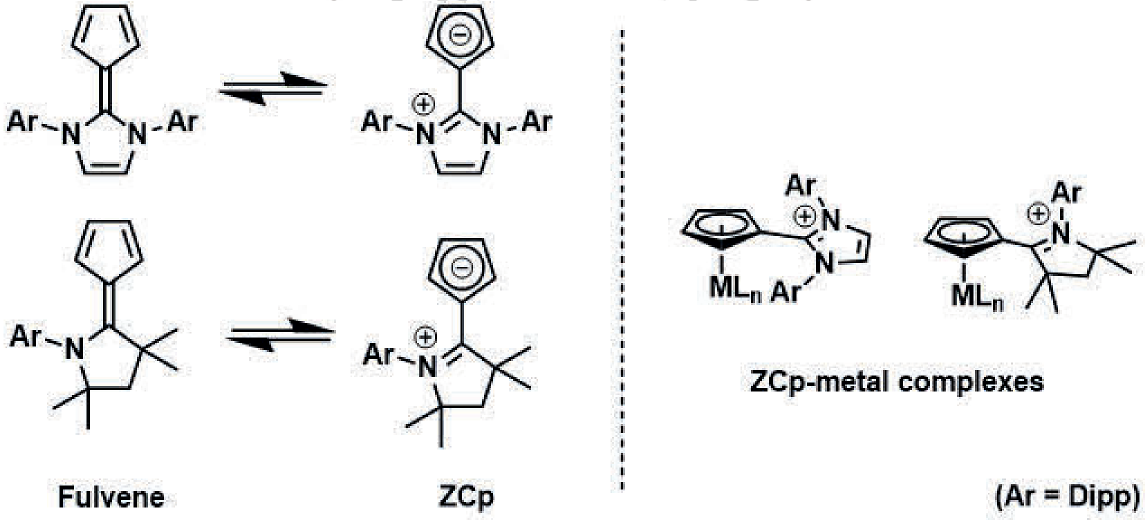
Poster Presentation : **INOR.P-146**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Imidazolium-/Pyrrolinium-substituted Zwitterionic Cyclopentadienyl Derivatives

Hyeonjeong Choi, Hayoung Song[1], Eunsung Lee[1,*]

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

The one-electron reduced ferrocene, ferrocenate, is generally known to be unstable due to its fast dissociation of cyclopentadienyl anion (Cp) from iron. However, our group reported a study that the ferrocenate can be stabilized at room temperature by introducing pyrrolinium and imidazolium moieties as substituents on the Cp ligand, recently. The substituted Cp has zwitterionic property and shows the ability to stabilize low-valent metal by serving as a redox-active ligand. From previous studies, we noted the general utility of zwitterionic Cp derivatives (ZCp). In this study, first, we introduce a synthesis of new ZCp which are fulvene derivatives with neutral properties. Their structural and electronic properties are also characterized by NMR, SCXRD and UV-Vis. Additionally, the ZCp-metal complexes were also synthesized and characterized.



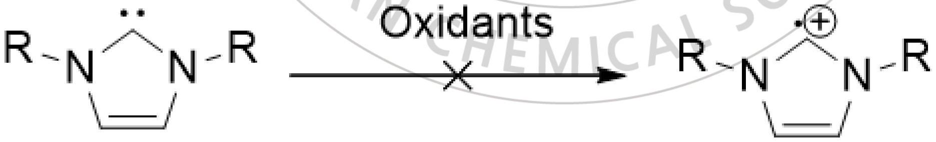
Poster Presentation : **INOR.P-147**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Can N-heterocyclic carbene be used as a reducing agent?

Hayoung Song, Eunsung Lee*

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

The high nucleophilicity of N-heterocyclic carbenes (NHCs) has enabled various applications of NHCs such as organocatalysts and ligands of transition metal complexes. Their high sigma-electron donating property raised expectations for the potential application of NHCs as reducing agents. While several examples have been reported to apply NHCs as reducing agents, the direct evidence of single-electron transfer (SET) from NHC to other electrophiles has not been reported so far. Recently, Severin group reported that the direct observation of SET from NHC to tritylium and also confirmed the decomposition of the transient intermediates generated by the SET process.However, the oxidation of NHC is highly challenging due to the electronegativity of the nitrogen atom on the carbene center. Reproducing existing studies on NHC oxidation, we confirmed that the existing studies are misleading. In this presentation, we will point out and clarify the misunderstandings presented by previous studies on the oxidation of NHCs.



Poster Presentation : **INOR.P-148**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Fabrication of Bright Green InP/ZnSeS/ZnS Quantum Dot Embedded Spherical Al_2O_3 Powders

Seonwoo Ahn, Minji Ko[1], Young rag Do[1,*]

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

We introduce a simple and effective strategy for quantum dot (QD) uniformly embedded spherical Al_2O_3 powders through a combination of electro-spray (e-spray) and fast hydrolysis reaction of aluminum tri-sec-butoxide. Green InP/ZnSeS/ZnS was prepared using hot-injection method. After this, their surfaces were in-situ-treated with $Hf(OtBu)_4$ to protect against surface damage during the e-spray process. As-prepared $Hf(OtBu)_4$ -treated InP/ZnSeS/ZnS QDs were mixed with aluminum tri-sec-butoxide in toluene. The mixed solution was e-sprayed onto a glass substrate and QD embedded Al_2O_3 powders were obtained. Pristine $Hf(OtBu)_4$-InP/ZnSeS/ZnS QDs showed a photoluminescence quantum yield (PLQY) of 0.85 with a peak wavelength of 520 nm. $Hf(OtBu)_4$-InP/ZnSeS/ZnS@ Al_2O_3 beads showed photoluminescence quantum yield (PLQY) of 0.70 with a peak wavelength of 530 nm. SEM images of beads showed spherical QD@Al_2O_3 beads with average diameters of ~3 ㎛.

Poster Presentation : **INOR.P-149**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Tunable Ambiphilic N-heterocyclic Carbene: Coumaraz-2-on-4-ylidene (CONY)

Hayoung Song, Hyunho Kim, Eunsung Lee[*]

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

Recently, N-heterocyclic carbenes (NHCs) are used for many fields, such as activation of small molecules and ligands for transition metal complexes. NHC ligands are attract tools in ognanic and inogranic chemistry because of it's special electronic properties. Especially, the property that people have attention is σ-donor ability, which is most powerful among various ligands. So, the σ-donor properties of NHCs are unveiled so much, but the π-accepting properties(π-acidity) of NHCs are not studied well. To unveil the π-accepting properties of NHCs, we have synthesized new ambiphilic NHC, called Coumaraz-2-on-4-ylidene (CONY). This ambiphilic NHC still has strong σ-donor ability with strong π-accepting ability too. In addition, various kinds of precursors which affect to electronic properties of carbene ligands are synthesized by simple two steps with high yields. Their rhodium complexes and the specific reactivity of the CONYs were identified. Furthermore, CONY show extremely low LUMO energy level compared with other NHCs which was confirmed by experimental method (77Se NMR chemical shift of the selenium adducts) and DFT cacluation.

Poster Presentation : **INOR.P-150**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

The fabrication of GaN-based micro-light-emitting diode (LED) and chip individualization by dicing.

Selim Yun, SeungJe Lee, Yun Jae Eo[1], Eunha Hong, Young rag Do[*]

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

This work studies the fabrication of GaN-based micro-LED arrays and LED chips isolated by laser dicing. ITO was deposited on GaN grown on 4-inch patterned sapphire substrate (PSS). The lateral LED arrays were fabricated by using repeated photolithography, dry etching and deposition process. After that, wafer thickness has reduced by lapping process and LED chips individually separated by laser dicing process. We measured electroluminescence spectrum and I-V curve by using a probe station from 0.1mA to 50mA. We expect that GaN-based LED chips aligned using appropriate transfer technology can be applied to various areas of the display industry.

Poster Presentation : **INOR.P-151**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Enhanced efficiency of Molybdenum Cu-In-Ga-Se (CIGS) Solar Cells according to Direct or Indirect Patterning

Hyengjin Kim, SeungJe Lee, Young rag Do[1,*]

Department of Chemistry, Kookmin University, Korea

[1]*Department of Bionano Chemistry, Kookmin University, Korea*

There are many different ways to perform pattern processes in nano units. Various processes are being developed, such as a photo process using photo-lithography, soft-lithography using a soft stamp, and transfer patterning of nano size to the substrate. Among these, patterning using nano-imprinting processing methods can make it relatively easy to pattern large areas and to increase the efficiency of Cu-In-Ga-Se (CIGS) solar cells using molybdenum in patterning. The patterning method we will introduce here is to use the nano-imprinting process with the spin-on-glass (SOG) as an imprint resin. Spin-on-glass (SOG) can perform curing using O_2 plasma without a separate heat curing or UV curing process. It is possible to improve power conversion efficiency (PCE) for CIGS solar cells by implementing indirect and direct patterning.

Poster Presentation : **INOR.P-152**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Hydrochromic application of Diphiylleia grayi-inspired PDMS film

SeungJe Lee, Minji Ko, Hyengjin Kim[1], Young rag Do[2,*]

Department of Chemistry, Kookmin University, Korea
[1]*applied chemistry, Kookmin University, Korea*
[2]*Department of Bionano Chemistry, Kookmin University, Korea*

In the fields of anti-counterfeiting, security codes, and sensors, various hydrochromic and electrochromic applications have been developed. Among these methods, applications using the hydrochromic property showed high energy efficiency because large energy was not required for color conversion. Diphylleia grayi, a flower that turns transparent when it rains, inspired hydrochromic applications. In this study, a new type of hydrochromic film was fabricated by forming a nanocavity structure on the surface of a PMDS film and patterning it with an inverse opal array using the nanosphere transfer method. The difference in contrast ratio between wet and dry states was measured using nanospheres of various cycles. Among them, the 1μm nano cavity structure film exhibited the largest contrast ratio. The difference between the diffusive transmittance and the transmittance values in the dry and wet conditions in the hydrochromic film showing the largest contrast ratio were as follows: (44.93% (ΔTD) T = 59.11–14.18%) and 54.88% (ΔH = 69.42–14.54%). The dynamic water modulation of the scattering opaque and non-mixing transparent states of these nano cavity structure PDMS films can provide an advanced platform structure in the area of hydrochromic technology for smart windows, camouflage, and transparent umbrellas on rainy days.

Poster Presentation : **INOR.P-153**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Cs3MnBr5 phosphor through solid state method

Sang wook Park, Keyong Nam Lee, Young rag Do[1,*]

Department of Chemistry, Kookmin University, Korea
[1]*Department of Bionano Chemistry, Kookmin University, Korea*

Research is ongoing to find an eco-friendly alternative material because lead, a synthetic material, has problems in terms of eco-friendliness. Perovskite nanocrystals, such as cesium lead halide, are potential emissive materials in the lighting and display field. However, cesium lead halide perovskites have the following problem. The material lead (Pb), used to synthesize cesium lead halide perovskites, is toxic to humans. Therefore, research for perovskites based on eco-friendly and alternative materials is important. Recently, in some papers, Cs3MnBr5 has usually been synthesized through ionization-recrystallization or hot injection method. In this study, we used solid-state chemistry to synthesize Cs3MnBr5 phosphor. We observed that a light green powder had been synthesized. The photoluminescence quantum yield (PLQY), emission wavelength, and full width at half-maximum (FWHM) of green emissive phosphor were 36%, 525 nm, and 41 nm.

Poster Presentation : **INOR.P-154**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Structural Analysis of Heteroleptic Molybdenum Complex using *N*-Alkoxy Carboxamide Ligands

Sung Kwang Lee, Bo Keun Park, Seung Uk Son[1], Taek-Mo Chung[2,*]

Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*
[2]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

Generally, metal elements have good electrical conductivity and have been used in various fields by atomic layer deposition (ALD) process. Some metals are using as precursor for semiconductor or display process. Molybdenum is 6-group transition metal and has high melting point, good thermal stability, low resistivity. Because of its characteristics, it can be used as good diffusion barrier when it is deposited. Molybdenum must be formed coordination complexes with various ligands to deposit molybdenum (Mo), molybdenum nitride (MoN_x) or molybdenum oxide (MoO_x) films on substrate. Especially, molybdenum oxide has been used in metal-oxide semiconductor, gas sensor, or some optical devices. For this applications, imido ligand (*tert*-butylamine) and *N*-alkoxy carboxamide ligands are used for heteroleptic molybdenum complexes. Each ligands have oxygen or nitrogen-coordinating sites, so complexes can be deposited as molybdenum oxide thin film by ALD process.Molybdenum complexes were synthesized by reacting $Mo(N^tBu)_2Cl_2$ with sodium-substituted *N*-alkoxy carboxamide ligands in hexane. Newly synthesized molybdenum complexes were characterized by single crystal XRD analysis, ^1H NMR spectroscopy, elemental analysis, and thermal stability of complexes was investigated by TGA. $Mo(N^tBu)_2(mdpa)_2$ (mdpaH = *N*-methoxy-*2,2*-dimethylpropanamide) is existed in a distorted octahedral, where molybdenum metals have 6-coordination bonds of nitrogens and oxygens from imido and carboxamide ligands.

Poster Presentation : **INOR.P-155**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis Method of Mesoporous Silica with High Specific Surface Area through Room Temperature Process using Sodium Silicate Solution

MinKyoung Kim, **Jae Young Bae**[1,*]

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

This study synthesized mesoporous silica using sodium silicate solution at a room temperature synthesis method without heat treatment. Sodium silicate solution was used as a precursor of mesoporous silica, and a porous structure was realized by self-assembly with CTACl. After synthesis, CTACl of the porous silica was removed using EtOH/HCl, and the remaining CTACl was effectively eliminated during washing process. The synthesized mesoporous silica was compared and analyzed with the mesoporous silica made by a heat treatment process. Characterization was performed by FT-IR, TEM, TGA, N_2-sorption and XRD. According to the sodium silicate concentration during synthesis, we confirmed that the specific surface area was larger than 1,000 m^2/g.

Poster Presentation : **INOR.P-156**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Coordinative Equilibrium at Open Metal Sites in Metal-Organic Framework

Sun Ho Park, Nak Cheon Jeong*

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

Metal-Organic Frameworks (MOFs) are crystalline porous materials composed of metal ion nodes and multitopic organic ligands. In particular, MOFs with open coordination sites (OCSs) where Lewis-base guest molecules can form coordination bonding often function an important role in potential applications such as catalysis, gas absorption, gas separation, drug delivery, chemical sensing, electronics, and ionic conduction. Although OCSs are a significant factor in these applications, but the study of the coordination nature of the OCSs remains a challenging issue. Meanwhile, a neutral chlorine atom molecule, trichloromethane (TCM), is known to be polar but non-coordinating. In this study, we have observed weak coordination ability of TCM to use MOFs as a platform via monitoring real-time in situ NMR and Raman studies. Because of these studies, we propose a new concept of “coordinative equilibrium” that is formed via coordination exchange between strong-basic molecules (e.g., H_2O, MeOH, EtOH, DMF, and phenol) and weak Lewis-basic molecules TCM.

Poster Presentation : **INOR.P-157**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Characterization of New Nickel-Bismuth Pincer Complexes

Dagyum Yoo, Yunho Lee[*]

Department of Chemistry, Seoul National University, Korea

Developing new catalysts with high economic advantages using 1st row transition metals are currently drawing attention. Despite being inexpensive and abundant, such 1st row transition metal complexes are not widely used in industry due to their limited applications. Controlling the properties of 1st row metals to mimic the intrinsic character of the frontier orbitals of heavy 2nd and 3rd row metals would expand its utility. As a new synthetic methodology, metal-ligand cooperation (MLC) has been employed to tune the chemical properties of the light transition metals. In this study, we synthesized a series of new bismuth-nickel pincer complexes based on a bismuth-containing tetradentate ligand (BiP_3) to explore the reactivity of the Bi–Ni site. From a BiP_3 ligand, the oxidative-addition of a Bi–C bond at nickel(0) species gave a distorted trigonal bipyramidal nickel(II) complex, $(BiP)_2Ni(PPh)$. Reaction of this nickel(II) complex with MeI also gave the oxidative-addition product, $(BiP_2Me)Ni(I)(PPh)$, where methylation occurs at the Bi site and nickel gets oxidized by 2-electrons. Subsequential exposure with UV-irradiation, resulted in the four-coordinate reduction product, $(BiP_2)Ni(I)$ possessing highly distorted square planar geometry with a shortened Bi–Ni bond length compared to those of $(BiP)_2Ni(PPh)$. As an alternative way to prepare a metal-halide complex, HCl was directly reacted with $(BiP)_2Ni(PPh)$ to give $(BiP_2)NiCl$. It was previously reported that tBuNC could induce migration of a nickel-bonding moiety to the central phosphide moiety of a PP_2 ligand. Here, we treated $(BiP_2)NiCl$ with tert-butyl isocyanide, resulting in the formation of a trigonal bipyramidal species, $\{(BiP_2)Ni(tBuNC)_2\}\{Cl\}$. Interestingly, the chloride anion weakly interacts with bismuth, showing an unprecedently long Bi–Cl bond length of 3.16 Å causing Bi–Ni bond to be elongated. The resulting product, $[(BiP_2)Ni(tBuNC)_2][BPh_4]$, was synthesized by the addition of $NaBPh_4$ to the $\{(BiP_2)Ni(tBuNC)_2\}\{Cl\}$. The product showed shorter Bi–Ni bond length of 2.617(1) Å than those of the starting material. This work provides information on the bonding character of two metal sites, bismuth and nickel, as well as the reactions occurs in a heterobimetallic cooperative way of a Bi–Ni site.

Poster Presentation : **INOR.P-158**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Suppressing thermal conductivity of SnTe by fluidic interstitial Cu atoms

Jaeho Lee, Chung In[1,*]

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

SnTe is a lead-free thermoelectric material of which maximum power conversion efficiency is achievable in the intermediate temperature range of 600-900K. It is a promising less toxic alternative to PbTe. In contrast to PbTe, SnTe has been ignored for thermoelectric applications because of too high thermal conductivity mainly due to the high hole concentration arising from inherent Sn vacancies in the lattice, very small band gap (~0.18 eV) and a large energy split between light-heavy hole valance bands. As a result, its thermoelectric figure of merit (ZT) has been limited to ~0.5 at 873K. In this presentation, we demonstrate thermal conductivity of SnTe can be substantially suppressed down to ~1.2W/mK at 873K by incorporating fluidic Cu atoms into the interstitial voids of the SnTe lattices. Consequently, the best composition sample exhibits a ZT ~1.5 at 873K.Keywords: SnTe, thermal conductivity, liquid like behavior, ZT

Poster Presentation : **INOR.P-159**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Diphenyl-Substituted Acridane PNP LigandPlatform for Small Molecule Activation

Lecita Bowen, Yunho Lee[1,*]

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

As a key technology for the carbon neutral industry, the conversion of CO_2 into industrially important products has been of keen interest in recent years. In particular, CO_2 conversions mediated by transition metal complexes continue to attract much attention because various value-added products can be generated from CO_2 as a C1 source. Our group has explored the chemistry of low-valent nickel supported by pincer systems. We first investigated the flexible PNP ligand, and reported the reaction of the zerovalent nickel complex {Na}{(PNP)Ni(CO)}, with CO_2. Due to the nucleophilicity of the central amido nitrogen of the PNP ligand, its reaction with CO_2 resulted in the generation of multiple products, including a tetrameric cluster complex. This suggested that competition might occur between the nickel ion and the amido nitrogen during the reaction. Recently, we also reported a new acriPNP pincer ligand (acriPNP$^-$ = 4,5-bis(diisopropylphosphino)-2,7,9,9-tetramethyl-9H-acridin-10-ide), and its nickel complexes. This rigidified (acriPNP)Ni scaffold showed a unique result, markedly different from the flexible analogous PNP ligand. Upon addition of CO_2 to the nickel(0)–CO species, a nickel(II) carboxylate species, with a Ni(η^1-CO_2-κC) moiety, was successfully formed. This selective CO_2 reaction implies that the methyl groups of the ligand, in the secondary coordination sphere, play a role in suppressing the competing reaction. We further modified the PNP ligand to prepare the ^{Ph}acriPNP pincer ligands, where ^{Ph}acriPNP$^-$ = 4,5-bis(X_2phosphino)-3,6-dimethyl-9,9-diphenyl-9H-acridin-10-ide (X = Cy or iPr), and explored the reactivity of their low-valent nickel carbonyl species towards CO_2. We believe that the bulkier phenyl groups would provide better steric shielding of the amido nitrogen. These results regarding a new strategy for small molecule conversion, mediated by a low valent nickel ion supported by a structurally rigidified ligand scaffold, will be discussed.

Poster Presentation : **INOR.P-160**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis, characterization and catalytic activity of a mononuclear nonheme copper(II)-iodosylbenzene adduct

Hyeri Jeon, Hanae Lim, Hyungbin Park, Seungwoo Hong*

Department of Chemistry, Sookmyung Women's University, Korea

Iodosylbenzene (PhIO) and its derivatives have attracted significant attention due to their various applications in organic synthesis and biomimetic studies. For example, PhIO has been extensively used for generating high-valent metal-oxo species that have been regarded as key intermediates in diverse oxidative reactions in biological system. However, recent studies have shown that metal-iodosylbenzene adduct, known as a precursor of metal-oxo species, plays an important role in transition metal-catalyzed oxidation reactions. During last few decades, extensive investigations have been conducted on the synthesis and reactivity studies of metal-iodosylbenzene adducts with early and middle transition metals including manganese, iron, cobalt. Nevertheless, metal-iodosylbenzene adducts with late transition metals such as nickel, copper and zinc, still remains elusive. Herein, we report a novel copper(II)-iodosylbenzene adduct bearing a linear ligand composed of two pyridine rings and an ethoxyethanol side-chain, $[Cu(OIPh)(HN3O2)]^{2+}$ (**1**). The copper(II)-iodosylbenzene adduct was characterized by several spectroscopic methods including UV-vis spectroscopy, electrospray ionization mass spectrometer (ESI MS), and electron paramagnetic resonance (EPR) combined with theoretical calculations. Interestingly, **1** can carry out the catalytic sulfoxidation reaction. In sulfoxidation reaction with thioanisole under catalytic reaction condition, not only two-electron but also four-electron oxidized products such sulfoxide and sulfone were yielded, respectively. However, **1** was not an efficient oxidant towards C–H bond activation and epoxidation reactions due to the steric hindrance created by the intramolecular H-bonding interaction between HN3O2 ligand and iodosylbenzene moiety.

Poster Presentation : **INOR.P-161**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

[Withdrawal] Extending photoluminescence lifetime of long lived exciton in organic-inorganic hybrid materials by triplet energy transfer

Dawoon Kim, Chung In[1,*]

School of Chemical and Biological Engineering and Center for Correlated Electron Systems, Institute for Basic Science (IBS), Korea

[1]*School of Chemical & Biological Engineering and Center for Correlated Electron Systems, Institute for Basic Science (IBS) , Korea*

Poster Presentation : **INOR.P-162**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Zintl Analogue of 2D Materials with High Carrier Mobility

Weiqun Lu, Chung In[1,*]

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

Since the pioneering studies in 2004, graphene, opening the rapidly emerging field of 2D materials, provides a flexible platform to study the structure–property correlation. Inspired by the success of graphene, alternative growing members are constantly being created for their potential applications. Here we have systematically evaluated the phase evolution of three Zintl zinc antimonides. In particular, the lamellar ZnSb phase with the sp2 hybridization has weak van der Waals forces in the interlayer region, associated with exfoliation availability. The stacking sequence of constituent atoms observed by the aberration-corrected STEM images also confirms its exfoliatable feature. Notably, layered ZnSb (2D) exhibits high carrier mobility up to ~468 cm2 V−1 s−1 at room temperature, more than 5 times that of the 3D ZnSb phase, equivalent to or even higher than those of the other representative 2D materials. The research reported here casts light on synthesizing novel 2D materials through stepwise topotactic approaches with unpredictable physical characteristics.

Poster Presentation : **INOR.P-163**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Deciphering Ancillary Ligand Effects on the O2-Activation by Nonheme Iron Enzyme Model Complexes

Hyungbin Park, Hyeri Jeon[1], Hanae Lim[1], Seungwoo Hong[1,*]

Department of Chemistry , Sookmyung Women's University, Korea
[1]*Department of Chemistry, Sookmyung Women's University, Korea*

A series of non-heme oxo-bridged diferric complexes, [Fe2(μ-O)(HN3O2)2]2, [Fe2(μ-O)(HN3O2)2(Cl)2]2+, [Fe2(μ-O)(HN3O2)2(NCS)4]2+ and [Fe2(μ-O)(HN3O2)2(N3)4]2+ where HN3O2 = 2-2-(bis(pyridine-2-ylmethyl)-amino)ethoxy)ethanol, have been isolated and characterized using various spectroscopic techniques including X-ray crystallography. While these complexes possess a distorted bioctahedral geometry in which each iron atom is coordinated to an oxygen atom of the μ-oxo bridge, the presence of ancillary ligands changed their inner sphere coordination manner; labile ethoxyethanol side chain could be replaced by ancillary ligands. This structural change in the coordination sphere greatly affects their electrochemical properties and influences the O2-activation reaction rates. These results provide interesting aspects of O2-ativation processes that can be modulated and controlled by the presence of diverse ions present in the biological system.

Poster Presentation : **INOR.P-164**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Preparation of core-shell Fe_3O_4@Polydopamine@UiO-66 and its catalytic properties in the degradation of chemical warfare agent simulant with IR irradiation.

Woon Jin Jang, Suk Joong Lee*

Department of Chemistry, Korea University, Korea

The rapid development of chemical warfare agents (CWA) threat to public safety and numerous detoxification studies of CWA have been widely conducted. In particular, Zr-based metal-organic frameworks(MOFs), such as UiO-66, are attracting much attention due to their high catalytic activity towards various CWAs, G- and V- series of nerve agents. Generally, CWA can be classified into three different series, G, V and H. G series is Tabun (GA), Sarin (GB), Soman (GD) and Cyclosarin (GF). V-series is VX, VR and VP. H-series are Sulfur mustard (HD) and Nitrogen mustard (HN). In particular, the nerve agent is one of the most fatal CWAs and causes serious casualties in a very small amount in a short time.Herein, we report a three-layer core-shell structure catalyst to improve the catalytic effect of MOFs. The outermost layer is a MOFs, in which a catalyst decomposes CWA which is prepared by a layer-by-layer epitaxial growth strategy. The layer below the MOFs is made of poly-dopamine, which receives IR LED light or sunlight to generate high heat and transfers it to the MOFs to increasing the efficiency of the catalyst. Lastly, the core of the catalyst consists of iron oxide, this magnetic core helps to easily recover the catalyst after use and easy to build up the MOFs layer

Poster Presentation : **INOR.P-165**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Photothermally Enhanced Catalytic Activity of Metal Oxide Composites for Detoxification of Chemical Warfare Agent (CWA) Simulant

Ye Ji Kim, Suk Joong Lee*

Department of Chemistry, Korea University, Korea

Many researches focus on the destruction of chemical warfare agents (CWAs) such as nerve, blister, choking, and blood agents. Especially, the organophosphate compounds VX, sarin (GB), and tabun (GA) are the main fatal agents which can cause permanent damage. Metal oxides have been investigated as catalysts for the detoxification of such agents. They usually provide a Lewis acid site and allow the reaction to take place easily. This type of reaction may take place quickly with a high reaction temperature. In this regard, we have introduced graphene oxide to control the reaction temperature by IR irradiation. Metal oxide nanoparticles which have a large ratio of surface area/unit volume were attractive as the catalyst. Mesoporous silica has been used as support for the metal catalysts to disperse them. Therefore, we can prevent agglomeration by incorporating metal oxide nanoparticles into the well-ordered pores of mesoporous silica. However, metal oxides have the drawback of relatively low catalytic activity. To enhance the reaction rate, we increased the reaction temperature via the near-infrared photothermal effect of graphene oxide. Here, we successfully synthesized the metal oxide composites and decomposed the nerve agent simulant with improved reactivity.

Poster Presentation : **INOR.P-166**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Differences in fraction and reactivity between Au precursors govern the synthetic mechanism of thiolate-protected Au nanoclusters

Ji Soo Kim, Sungsu Kang, Jungwon Park*

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

In colloidal synthesis of inorganic nanoparticles, all chemical reactions initiate from the precursors containing metal atoms. Their reactivity can directly affect the entire aspects of synthetic process including the reaction kinetics, and the homogeneity of final products. Gold nanoclusters (Au NCs) are a special class of nanoparticles in that they are produced by the slow reduction from the special precursors, Au(I)-SR complexes. Though the reduction process from the Au(I)-SR complexes to Au NCs has been delicately examined by controlling the reduction power, studying such process in terms of controlling the complexes as precursors is less assessed. Herein, we reveal that controlling the fraction of Au(I)-SR complexes can directly govern the reaction mechanism of Au NCs. The strong Au-S bond regulates the reactivity of Au(I)-SR complexes of which high amount leads to decelerate the reduction kinetics and maintain the homogeneity of produced Au NCs. Also, we hypothesize that Au(I)-SR complexes can have different reactivity by their degree of Au-S bond, which renders the specific complexes act as an actual precursor to Au NCs. Such claims are supported by various characterizations including UV-Vis absorbance, MALDI-TOF-MS, aberration-corrected TEM, and EXAFS.

Poster Presentation : **INOR.P-167**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Graphitization of amorphous carbon enabled by Magnesiothermic Reduction of SiO2@C to Si@C

Hyun Choi, Min Seok Kang[1], Chanyoung Lee, Won Cheol Yoo[2,*]

Department of Applied chemistry, Hanyang University, Korea
[1]*Department of Applied Chemistry, Hanyang University, Korea*
[2]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*

Magnesiothermic reduction of silica to silicon (SiO2 + 2Mg -> Si + 2MgO) has been widely employed to produce valuable silicon from abundant and cheap silica source. Due to a high reduction potential of Mg, this exothermic reaction releases a large amount of heat during the reaction. In this presentation, we elucidate the graphitization of amorphous carbon caused by the exothermic heat released during magnesiothermic reduction of SiO2@C, resulting in silicon@graphite (Si@G). Various physicochemical techniques were employed for proving this transformation that local graphitization of amorphous carbon was clearly identified. Furthermore, Si@G was employed as an anode for lithium-ion batteries that graphitized carbon shell effectively mitigated a large volume change of Si during electrochemical cycle, delivering a high capacity larger than 1000 mAh/g and outstanding long-term cycling performance.

Poster Presentation : **INOR.P-168**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Ge(β-diketonate)(N-alkoxy carboxamide) Complexes for Thin Film Application

<u>Heenang Choi</u>, Bo Keun Park[1], Seung Uk Son[2], Taek-Mo Chung[3,*]

Thin Film Materials Research Group, Korea Research Institute of Chemical Technology, Korea
[1]*Thin Film Materials Research Center, Korea Research Institute of Chemical Technology, Korea*
[2]*Department of Chemistry, Sungkyunkwan University, Korea*
[3]*Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea*

Germanium materials have applications in various areas such as electronics, optical, laser and semiconductors. Especially, $Ge_2Sb_2Te_5$ (GST) is used as phase-change random access memory (PRAM) devices. Metal precursors for atomic layer deposition (ALD) and chemical layer deposition (CVD) are needed for suitable deposition of conformal films in the high aspect ratio trench and via structures for high-density memory devices.We have focused on the synthesis of new germanium precursors which can be applied to grow germanium-containing thin films by ALD/ CVD. The series of novel germanium (II) precursors have successfully synthesized containing the β-diketonate and N-alkoxy carboxamide ligands. These complexes were stabilized by chelating effect and coordination ability of each ligand that is β-diketonate and N-alkoxy carboxamide. All the synthesized complexes were characterized by XRC and NMR, FT-IR spectroscopy, elemental analysis, mass spectrometry as well as thermo-gravimetric (TG) analysis. Especially, the single-crystal X-ray diffraction studies of the corresponding complexes revealed that they crystallized in the monoclinic space group as monomers. Newly synthesized germanium complexes showed properties of high volatility and thermal stability, and could be potentially served as precursors for thin-film applications.

Poster Presentation : **INOR.P-169**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Copper-based zeolitic imidazolate frameworks and their gas sorption properties

CheolWon Jung, Geonryong Kim[1], Jaheon Kim[*]

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

We synthesized two porous zeolitic imidazolate frameworks (ZIFs) (termed Cu-ZIF-1 and Cu-ZIF-2)by the solvothermal reactions between copper salt and 2-nitroimidazole, respectively. Crystalstructures indicate that the Cu-ZIFs have severely flattened tetrahedral Cu(II) ions with two axial nitroO atoms located at distal positions, giving rise to three-dimensional GIS (Cu-ZIF-1) and RHO (Cu-ZIF-2) topology, respectively. The Cu-ZIFs are stable in air and even in acidic and basic aqueoussolutions. Cu-ZIF-1 has very narrow 2.6 Å channels that do not allow N_2 gas adsorption. In contrast, Cu-ZIF-2 has large 2.0 nm lta-type cages and high permanent porosity with a BET surface area of 1568 m^2/g and a pore volume of 0.64 cm^3/g. The total amounts of gas uptake at 298 K are 72 cm^3/g (8.5 MPa) for H_2, 154 cm^3/g (8.5 MPa) for CH_4, and 227 cm^3/g (5.1 MPa) for CO_2, respectively. We will also discuss the synthesis of other types of copper-based ZIFs.

Poster Presentation : **INOR.P-170**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis, crystal structures, and porosity of three-dimensional zinc-imidazolate-sulfate frameworks

Kyungkyou Noh, Yujin Kim[1], You Jin Oh[1], Jaheon Kim[1,*]

Department of Information Communication Convergence Technology, Soongsil University, Korea
[1]Department of Chemistry, Soongsil University, Korea

We could incorporate sulfate ions into ZIFs to produce three-dimensional zinc-imidazolate-sulfate frameworks (ZISFs): ZISF-1 and ZISF-2. ZISF-1 formulated as $(NH_2Me_2)[Zn(nIm)(SO_4)]$ (nIm = 2-nitroimidazolate) exhibits zeolite GIS topology. The cages are filled with dimethylammonium ions, resulting in no solvent-accessible pores. In contrast to ZISF-1, ZISF-2 has open pores between honeycomb-type layers composed of $Zn_6(nIm)_6$ 6MRs that are linked by sulfate ions. These layers are further connected with octahedral zinc ions through the oxygen atoms of the sulfate linkers. Interestingly, the pillar Oh Zn^{2+} ions could be replaced with external Ni^{2+} ions. The measured BET surface areas for ZISF-2 and ZISF-2(Ni) were 340, and 101 m^2/g respectively by N_2 adsorption measurements. ZISF-2 and ZISF-2(Ni) have permanent porosity confirmed by N_2 adsorption measurements.

Poster Presentation : **INOR.P-171**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and structural analysis of unsymetry heteroleptic strontium complexes

Chanwoo Park, Taek-Mo Chung[1,*]

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

Strontium was applied to variety field such as computer memory, superconductors, lectroluminescent films and mixed-electronic ionic conductors for fuel cell electrolytes. All of these application have required the fabrication of strontium containing oxide flims through ALD or CVD. For the deposition of thin films using these techniques, strontium precursors with good stability and volatility are essential. However, storontium has less soluble and poor volume properties, adequate ligand design and synthesis are required. We have studied variety stontium complexes and synthesized by reacting Sr(btsa)2(DME)2 with alkoxide and beta diketonate ligands. Synthesized strontium complexes were fully characterized by single crystal XRD analysis, H - NMR, elemental analysis, and thermal stability was analyzed by TGA. All complexes existed in unsymetric dimer complexes, where strontium metals have five coordination bonds of nitrogen and oxygens.

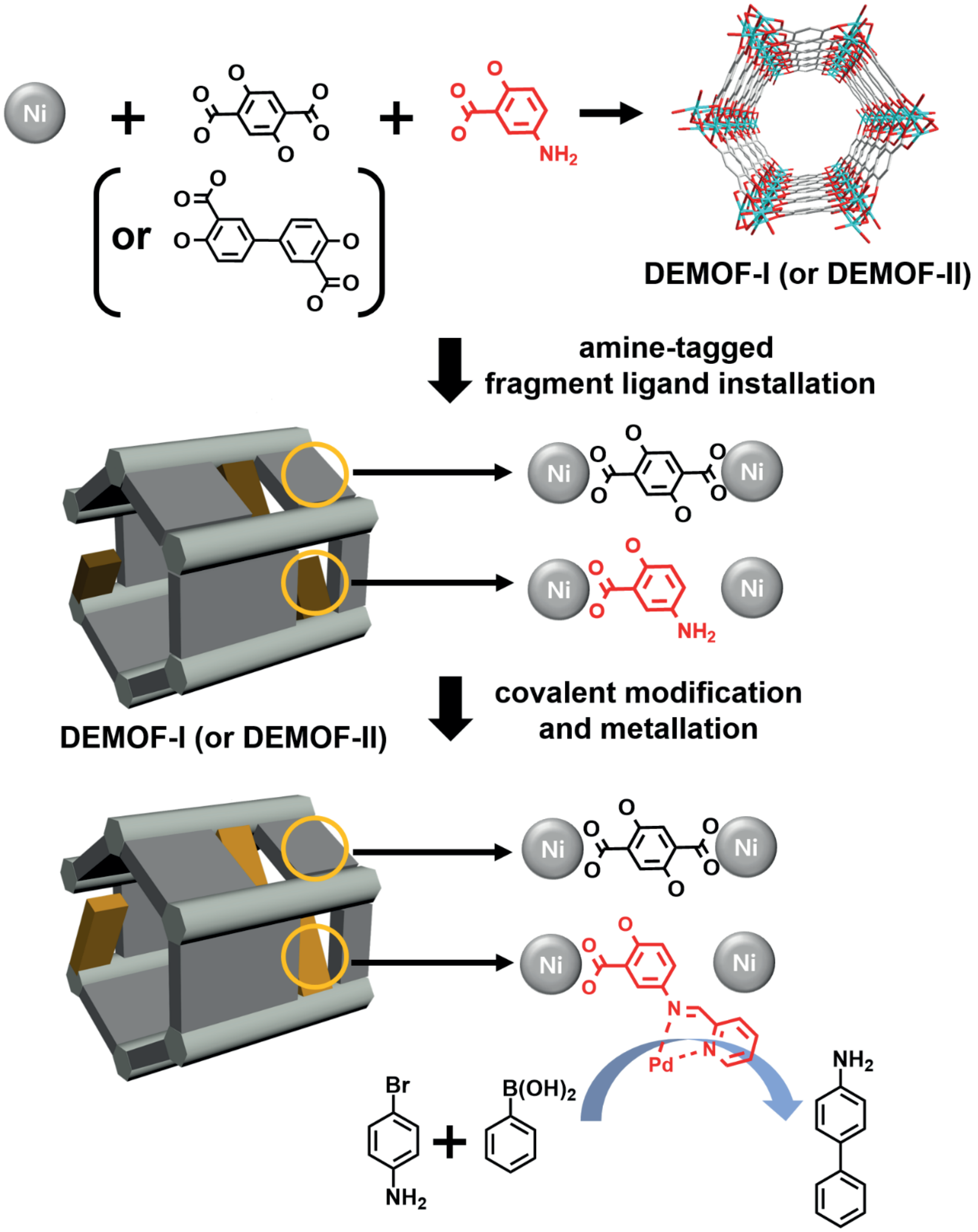
Poster Presentation : **INOR.P-172**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fragmented Ligand Installation for Covalent Modification of MOF-74

Jaewoong Lim, Min Kim[1], Myoung Soo Lah[*]

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

MOF-74 is one of the most explored metal-organic frameworks (MOFs), but its functionalization is limited to the dative post-synthetic modification (PSM) of the monodentate solvent site. Owing to the nature of the organic ligand and framework structure of MOF-74, the covalent PSM of MOF-74 is very demanding. Herein, we report, for the first time, the covalent PSM of amine-tagged defective Ni-MOF-74, which is prepared by de novo solvothermal synthesis using aminosalicylic acid as a functionalized fragmented organic ligand. The covalent PSM of the amino group generates metal-binding sites, and subsequent post-synthetic metalation with Pd(II) ions affords Pd(II)-incorporated Ni-MOF-74 catalyst. This catalyst exhibits highly efficient, size-selective, and recyclable catalytic activity for the Suzuki–Miyaura cross-coupling reaction. This strategy is also useful for the covalent modification of amine-tagged defective Ni2(DOBPDC), an expanded analog of MOF-74.


Ni
+
+
or
NH2
DEMOF-I (or DEMOF-II)
amine-tagged
fragment ligand installation
Ni
Ni
Ni
Ni
NH2
DEMOF-I (or DEMOF-II)
covalent modification
and metallation
Ni
Ni
Ni
Ni
N
Pd
N
Br
B(OH)2
+
NH2
NH2

Poster Presentation : **INOR.P-173**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

N-heterocyclic carbene difluoride sulfurane

Solhye Choe, Eunsung Lee[*]

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

The unique ability of sulfur-based fluorinating reagents such as DAST, XtalFluor, Fluolead has been extensively exploited in deoxygenative fluorination reagents for alcohols, aldehydes, ketones, and carboxylic acids. In 2015, Alcarazo group reported synthesis and reactivity of dihalo(imidazolium)sulfuranes that can transfer electrophilic groups, such as the CN group to organic nucleophiles. The cyanide group was further transferred to other compounds by C-H bond activation. Inspired by the work, we have been exploring the new deoxyfluorinating reagent based on N-heterocyclic carbene (NHC) by oxidation of NHC thioureas with xenon difluoride. It was characterized by NMR spectroscopy, elemental analysis, and X-ray crystallography. Synthetic methods and structural characterization of NHC-SF_2 will add to another important example of carbene intrinsic reactivity. This hypervalent sulfur was applied to NHC to deoxyfluorinate the carboxylic acid selectively, and additionally had different electronic properties in comparison to other sulfur-based deoxyfluorinating reagents.

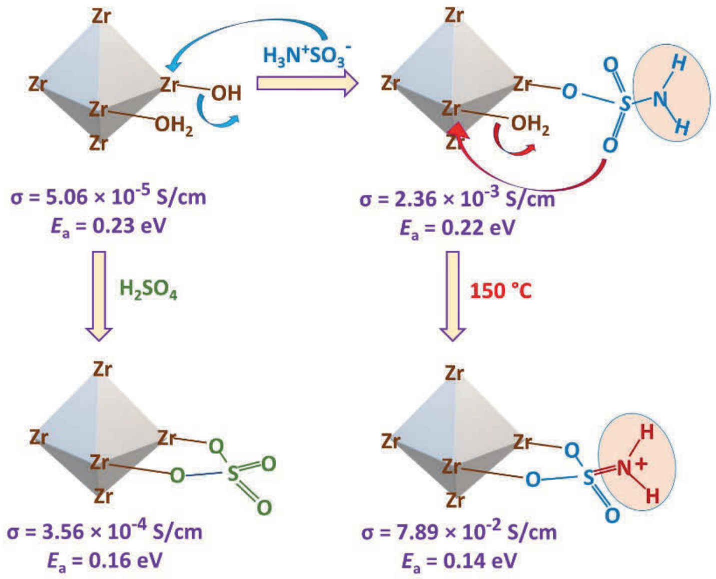
Poster Presentation : **INOR.P-174**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Superprotonic Conductivity of MOF-808 Achieved by Controlling the Binding Mode of Grafted Sulfamate.

Amitosh Sharma, Jaewoong Lim[1], Yung sam Kim[1,*], Myoung Soo Lah[1,*]

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

A metal–organic framework (MOF) having superprotonic conductivity, MOF-808, is prepared by modulating the binding mode of the sulfamate (SA) moieties grafted onto the metal clusters. The activation of the SA-grafted MOF-808 at 150 °C changes the binding mode of the grafted SA from monodentate to bridging bidentate, thus converting the neutral amido (–S–NH2) moiety of the grafted SA to the more acidic cationic sulfiliminium (–S=NH2+) moiety. Further, the acidic sulfiliminium moiety of MOF-808-4SA-150 results in more efficient proton conduction than the amido moiety of MOF-808-4SA-60. At 60 °C and 95% relative humidity, MOF-808-4SA-150 is found to have a proton conductivity of 7.89 × 10-2 S/cm, which is more than 30-times higher than that of MOF-808-4SA-60. Moreover, this superprotonic conductivity is well maintained over 1000 cycles of conductivity measurements and for similar cyclic measurements each day for seven days.


Zr
Zr
Zr
Zr
Zr
OH
OH_2
$H_3N^+SO_3^-$
σ = 5.06 × 10^{-5} S/cm
E_a = 0.23 eV
O
S
N
H
H
O
O
OH_2
σ = 2.36 × 10^{-3} S/cm
E_a = 0.22 eV
H_2SO_4
150 °C
σ = 3.56 × 10^{-4} S/cm
E_a = 0.16 eV
N+
σ = 7.89 × 10^{-2} S/cm
E_a = 0.14 eV

Poster Presentation : **INOR.P-175**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Tailoring extrinsic porosity of a metal-organic polyhedron

Kangwoo Jin, Jinhee Park[*]

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

Metal–organic polyhedra (MOPs) are intrinsically porous molecular materials, assembled via coordination bonds of organic linkers and metal nodes. One of the challenges most MOPs face is the blocking of pore windows by adjacent MOP molecules upon solvent removal. To overcome this problem, we rendered a microporous MOP into a hierarchically porous aerogel. The combined micro-to-macropores of the aerogels are potentially beneficial to many applications. Herein, the superiority of the MOP-based aerogel structure was demonstrated by being applied in chemical sensing applications. The vapochromic MOP was prepared in the forms of three polymorphs (amorphous powders, nanocrystals, and aerogels) with different porosities and their chemical sensing performances were successfully compared through visual detection of color changes upon vapor exposure.

Poster Presentation : **INOR.P-176**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Crystal structure and thermal stability of a new proton conducting material HTa_2PO_8

Junho Ha, Heeyoun Kim[1], Seung-Joo Kim[2,*]

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

The crystal structure and ionic conductivity of HTa_2PO_8, a new proton conducting material, are synthesized through a proton ion-exchange reaction on $LiTa_2PO_8$. HTa_2PO_8 is isotypic with $LiTa_2PO_8$. The protons occupy two different crystallographic sites in the void space of the $[Ta_2PO_8\ ]^-$ framework. This structures can be represented by the general formula $H(TaO_{6/2})_2(PO_{4/2})_1$, where the Ta and P atoms locate on the octahedral and tetrahedral sites, respectively. Conductivity measurements revealed that proton conduction is the main mechanism operative in HTa_2PO_8. Upon heating, HTa_2PO_8 decomposes via two steps as follows: $HTa_2PO_8 \rightarrow Ta_2PO_{7.5}$($T \approx 600$ °C) $\rightarrow 1/2Ta_2O_5 + TaPO_5$ ($T \approx 1050$ °C).

Poster Presentation : **INOR.P-177**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis, thermal redox reaction and catalytic activity of δ-$CaCr_2O_4$

Yewon Yoon, Fouzia Khefif, Seung-Joo Kim*

Department of Energy Systems Research, Ajou University, Korea

The thermal redox reactions of a Ca-Cr-O system under different atmospheric conditions were investigated by cyclic thermodiffractometry and thermogravimetry. Under a reductive atmosphere, $CaCrO_4$ decomposed into CaO and δ-$CaCr_2O_4$, with the liberation of free oxygen, under an oxidizing atmosphere, the reaction could proceed reversibly. δ-$CaCr_2O_4$ crystallized in a monoclinic structure (space group: $P2_1/m$). The structure can be described as a stacking of CrO_2 layers composed of edge-sharing CrO_6 octahedra, with calcium ions residing on-site between the layers. The calcium ions were coordinated by six oxygen atoms to form a trigonal prism geometry between the CrO_2 layers.The structure of δ-$CaCr_2O_4$ was distinct from those of low-temperature β-$CaCr_2O_4$ and high-temperature α-$CaCr_2O_4$ form. We also investigated the catalytic activity of δ-$CaCr_2O_4$ on the propane dehydrogenation reaction.

Poster Presentation : **INOR.P-178**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

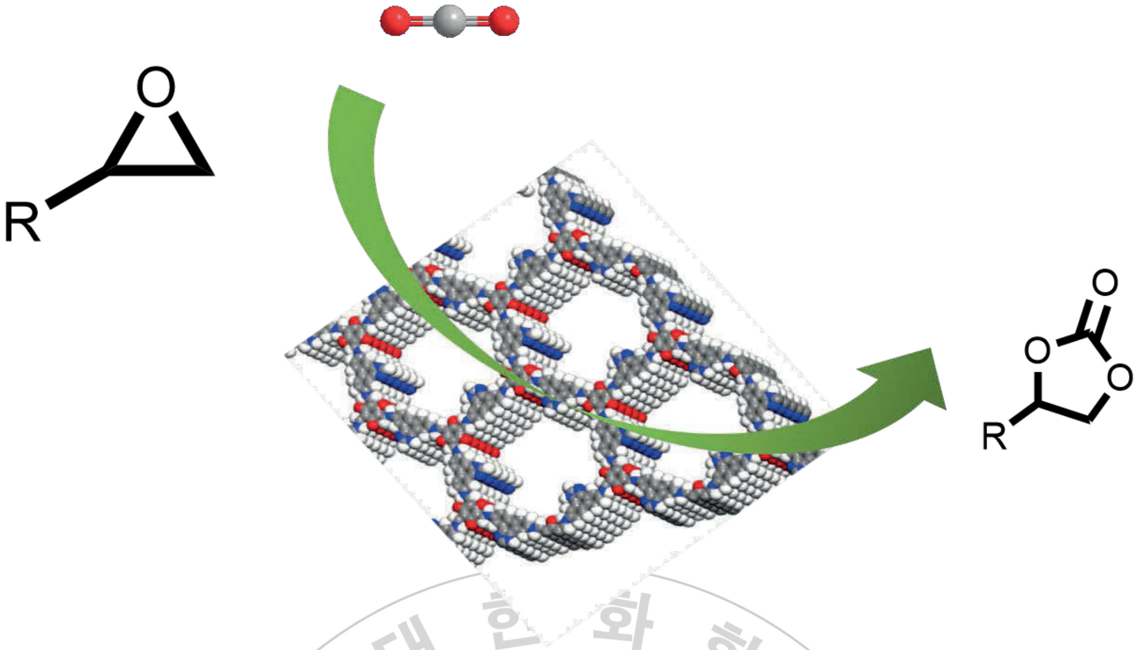
Construction of PIm-COFs as metal-free heterogeneous organocatalysts for chemical fixation of CO_2 under mild conditions

Congxue Liu, Eunsung Lee[1,*]

Chemistry, Pohang University of Science and Technology, Korea

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

Carbon dioxide is one of the main components of greenhouse gases, and the sharp increase in its content has had a particularly important impact on global warming. However, capturing and converting this inexpensive, readily available, non-toxic green carbon source into valuable chemicals which have always attracted the attention of scientists.Covalent organic frameworks (COFs) as a typical class of organic crystalline porous species have already been the most promising functional materials in gas adsorption and separation, energy storage, and catalytic organic transformation due to their crystalline network structure formed by organic building units and different topological structures.Herein, we report two phenanthro[9,10-d] imidazole-based COFs, which exhibit the outstanding adsorption of carbon dioxide. In addition, they possess ample reaction sites that successfully catalyst cycloaddition of CO_2 to epoxides under mild reaction conditions.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Poster Presentation : **INOR.P-179**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Electronic-Delocalization-driven Conductivity of Radical Anionic Ligand Stacks in Metal-Organic Frameworks

Seonghun Park, Jinhee Park[*]

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

Since Gomberg discovered a triphenylmethyl based organic radical, various types of organic radicals have been investigated due to their unique magnetic, electronic, optical, and redox properties. Among them, radical anions derived from 1,4,5,8-napnthalenediimide (NDI) and its derivatives have been widely explored for their applications such as in catalysis, photovoltaic cell, battery, and light-emitting devices. Due to a strong π-acidic property of NDIs, they are prone to being radical anions ($NDI^{\bullet-}$) and dianions (NDI^{2-}) via one- and two-electron transfers, respectively. Importantly, the radical states with the planar naphthalene moiety prefer to construct the infinite π stacks because through-space-electron-delocalization can stabilize the radical states. Herein, we successfully demonstrated that once the radical π stacks are incorporated into the metal-organic frameworks (MOFs) as an organic building block, the electronic conductivity of the MOFs can increase. Obtaining the radical anionic NDIs was a pre-requisite for synthesizing the π-stacks-based MOFs. This study will provide a deep insight into the role of the radical anionic species in forming π-stacks-based MOFs and their conductive behaviors.

Poster Presentation : **INOR.P-180**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Preparation of Fe-HKUST-1 via Mixing Metals *de novo* and Post-Synthetic Metal Metathesis

Asong Byun, Jinhee Park[*]

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

HKUST-1, consisting of 1,3,5-benzenetricarboxylates (BTC) and Cu^{2+}-paddle-wheel clusters, is one of the well-studied metal-organic frameworks (MOFs). While post-synthetic metal metatheses (PSMM) have been widely used for utilizing the structural characteristics of MOFs, the structural robustness of Cu-HKUST-1 prevents the PSMM. Herein, when the equal amounts of Cu^{2+} and Zn^{2+} are evenly distributed throughout the HKUST-1 networks, Zn^{2+} with the relatively weak bond easily falls off by other metal ions and Cu^{2+} with the stable bonds maintains the structure. Thus, the PSMM of Cu,Zn-HKUST-1 with Fe^{2+} can afford Fe-HKUST-1. Addition of a small amount of Fe^{3+} can accelerate the metathesis process.

Poster Presentation : **INOR.P-181**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Interpenetration of UiO-Type Metal-Organic Frameworks for Effective Catalysis

Sanghyeop Lee, Jinhee Park[1,*]

Emerging materials science, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1] *Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Metal-organic frameworks (MOFs), comprised of metal clusters and organic linkers, are an emerging class of porous and crystalline catalysts. Porosity increment is a general strategy to improve reagent accessibility to catalytically active sites and thus to enhance a catalytic activity. Thus, interpenetration of the independent frameworks, which decreases porosity, lowers catalytic performance. Herein, we synthesized three distinct Zr-based UiO-type MOFs with non-interpenetrated, partially-interpenetrated, and interpenetrated structures by carefully-regulating reaction conditions. When they are applied in an organic catalytic reaction, cyanosilylation, the interpenetrated structure exhibits the highest catalytic activity. Further examinations disclosed potential catalytic sites and possible mechanism, which offers a novel perspective for designing a highly active catalyst.

Poster Presentation : **INOR.P-182**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Bridging and Fixing Metal-Organic Polyhedra

Byeongchan Lee, Jinhee Park*

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

Metal-organic polyhedra (MOPs), composed of metal clusters and organic linkers, have attracted significant attention owing to their well-defined structures, intrinsic porosities, and solution processability. Tailored porous architectures of MOPs are attained through innumerable combinations of metal clusters and ligands, which leads to various applications such as gas separation, catalysis, sensing, and drug delivery. However, amorphization which is caused by a collapse of the MOP arrangements easily occurs during the desolvation process. As a result, the pore windows between neighboring cages are blocked, and the porosity of the MOPs is lost. In this work, we developed a strategy, bridging and fixing the MOPs, to retain the permanent porosity. Bridging the MOPs connects the cages by introducing covalent bonds through the electrophilic aromatic substitution of m-DOBDC ligands. The fixing process removes solvents strongly coordinated to the open metal site while maintaining the MOP arrangements. These two strategies can provide permanent porosities for the various MOPs, thereby increasing the utilization of the MOPs in various applications.

Poster Presentation : **INOR.P-183**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Dimeric Radical Anionic Naphthalene Diimides in a Metal-Organic Framework

Bongkyeom Kim, Jinhee Park[*]

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

Naphthalenediimides (NDIs) are well-known π-electron-deficient polycyclic aromatic compounds, capable of accepting and delocalizing electrons to reach radical anion (NDI•−) and dianion (NDI2−) states. Their optical, electronic, and magnetic properties can be tuned by the introduction of various functional groups on imide nitrogens or naphthalene core. These factors make NDIs a promising candidate in diverse fields such as molecular magnets, organic electronics, and photoelectrical devices. However, the inherent instability of NDI•− has impeded their practical applications. In this study, we proposed a novel NDI•− stabilization strategy: introduction of NDI dimers in a metal-organic framework (MOF) platform. The pristine DGIST-7 is composed of NDI•− which can be long-lasting in ambient conditions. The oxidized DGIST-7 was readily reduced into the radical states by various stimuli such as IR, visible light, UV, and heat. The stable crystallinity of DGIST-7 contributed to the crystallographic visualization of the structural transitions during the redox processes.

Poster Presentation : **INOR.P-184**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Nitrosyl Complexes at N-Heterocyclic Carbene Center

Junbeom Park, **Eunsung Lee***

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

N-Heterocyclic carbenes demonstrate wide application in various fields including catalysis, coordination chemistry, and main group chemistry. Especially, NHCs recently attracted the interests with their transition metal-like reactivity such as bond activation and ligand exchange. Nitric oxide is well-known to form various transition metal nitrosyl complexes. Due to noninnocent nature of nitric oxide as a ligand, transition metal nitrosyl complexes often possess several different structures and charge states. To describe complex electronic structures of such compounds, Enemark-Feltham notation $\{M–NO\}^n$ is widely used (n: total number of electrons in the metal d orbitals and π*(N–O) antibonding orbital).In 2015, our group reported that NHCs react with gaseous nitric oxide to afford radical adduct $[NHC–NO]^\bullet$, which is similar with transition metal nitrosyl complexes. In the context of NHC-metal similarity, we hypothesized that $[NHC–NO]^\bullet$ shows similar redox chemistry with $\{M–NO\}^n$ complexes. Here in, we introduce the redox chemistry of nitrosyl complexes at N-heterocyclic carbene center.

Poster Presentation : **INOR.P-185**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

NADH Regeneration Catalyzed by Hydride Species Induced from Bis-Carbene Rhodium Complex

Jennifer Juhyun Kim, Sungho Yoon*

Department of Chemistry, Chung-Ang University, Korea

In the field of enzymatic biotransformation, improving activities of catalysts in NADH regeneration is of pivotal interest. Carbene ligated rhodium complex, $[(\eta^5\text{-Cp*})Rh(MDI)Cl]^+$ (Cp* = pentamethylcyclopentadiene, MDI = 1,1'-methylenebis(3,3'-dimethylimidazolium)), was successfully synthesized and used as an efficient catalyst for the reduction of NAD^+ to NADH via hydride transfer reaction. Upon addition of formate to the water soluble complex, unprecedented and highly stable form of rhodium hydride intermediate, $[(\eta^5\text{-Cp*})Rh(MDI)H]^+$, was isolated. Reduction of NAD^+ to NADH was performed with TOF of 1,700 h^{-1} which was superior to the efficiency of the available $[Cp*Rh(bpy)Cl]^+$ catalyst.

Poster Presentation : **INOR.P-186**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis and characterization of nitrogen donor ligand and construction of 3D

Lee Hyemin, Haeri Lee[1,*]

Chemistry department, Hannam University, Korea

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

Bio-active molecules in nature, such as enzymes and anti-bodies, can be sorted out as supramolecules which are activated by binding guest molecules. To achieve designated functions, appropriate molecular design can be a key role in the introduction of molecular functions. In this research, we'd like to introduce nitrogen donor ligand and a series of isostructural coordination polymers were synthesized in self-assembly procedure.

Poster Presentation : **INOR.P-187**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Syntheses of New Cu(II) and Cu(I) Complexes for Direct Etherification Catalysts

Eun su Chae, Jang Hoon Cho, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

Etherification is an important organic reaction for making building blocks or polar aprotic solvents. Traditional etherification process, which known as Wiliamson ether synthesis, is well-known and simple method to synthesize ethers. But Wiliamson ether synthesis requires toxic organohalides or strong base to initiate S_N2 reaction that generates environmentally hazardous byproducts. For this reason, we have developed Cu(II)/Cu(I) complexes, which need only alcohols for initiating esterification reactions and preventing of side products. This new, direct etherification, reaction goes through alcohol dehydration by the Cu(II) and Cu(I) catalysts. In this study, we describes the synthesis of a new ligand, EbQMA (=(N*E*,N'*E*)-2,2'-(ethane-1,2-diyl)bis(N-(quinolin-8-ylmethylene)aniline)), and air stable copper complexes, [Cu(EbQMA)(THF)]I and [Cu(EbQMA)I]ClO_4. The identification of reaction products are also presented.

Poster Presentation : **INOR.P-188**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Iron- Catalyzed Carbon−Oxygen Bond Borylation of Aryl Methoxides

Jongheon Jeong, Eunsung Lee*

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

C(sp^2)–O electrophiles electrophiles have been shown to be reliable alternatives to aryl halides as coupling partners in the cross-coupling reactions due to the absence of toxic halogen byproducts, inertness, low cost, and ready availability. Recently, a series of transition metal-catalyzed cross-coupling reactions utilizing relatively reactive C–O electrophiles such as aryl sulfonates, phosphates, carbamates, or esters have been reported. However, using aryl methyl ether, one of the simplest and most atom-economical molecules among phenol derivatives, is still challenging, and only a few examples have been reported. This is probably ascribed to the high activation energy of C(sp^2)–OMe bonds and the poor leaving group ability of methoxy residues. But functionalization of C(sp^2)–OMe bonds is useful in organic synthesis because aryl methoxides are naturally abundant, non-toxic, and bench stable. In addition, due to their inertness toward already well-developed noble metal based cross-coupling reactions, developing practical catalytic fictionalization reaction of aryl methoxides can provide new synthetic strategies to give highly functionalized aryl compounds by orthogonal coupling. Organoboranes are widely used in synthetic and biomedical chemistry as building blocks because of their inertness, low price, ease of preparation, and tolerance for a variety of functional groups. Herein, an iron-catalyzed demethoxyborylation of aryl methoxides is described. This reaction can be carried out using the commercial iron salt and inexpensive ligand which can be easily synthesized in a single step without complicated isolation process. It shows high selectivity of C–OMe bonds over C–H bonds. Furthermore, we found that the reaction intermediate can be functionalized to build C–H, C–C, or C–Si bonds, which means our iron system can transform C–O bonds into diverse chemical bonds.

Poster Presentation : **INOR.P-189**
Inorganic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Supramolecular polymerization of Pt^{2+} complex with terpyridine-based ligand possessing in non-polar solvent

Minkyeong Hwang, Jong Hwa Jung[1,*]

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

We report on the supramolecular polymerization of Pt^{2+} complex with terpyridine-based ligand (**1**) possessing alanine moiety in nonpolar solvents. The supramolecular polymer **1-Pt** exhibited a strong orange emission as low as micromole concentration, which in nonpolar solvents. The supramolecular polymer **1-Pt** showed a typical fiber structure using scanning electron microscopy (SEM) observation. Moreover, A cooperative pathway involving a nucleation-elongation mechanism generated the supramolecular polymer **1-Pt**.

Poster Presentation : **INOR.P-190**

Inorganic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

[Withdrawal] Controllable synthesis of porous NiCo$_2$O$_4$/NiO nanostructures with tunable morphologies for lithium-ion batteries

Sudhakaran Moopri singer pandiyarajan, Hyun Choi[1], InCheol Heo[1], Won Cheol Yoo[2,*]

Chemical and Molecular Engineering, Hanyang University, India
[1]*Department of Applied chemistry, Hanyang University, Korea*
[2]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*

Poster Presentation : **PHYS.P-99**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Photo-physics of BODIPY

Sang Hak Lee*, One Heo

Department of Chemistry, Pusan National University, Korea

BODIPY (Boron-dipyrromethene) has been studied to understand its photo-physics and showed various optical applications due to their high quantum yield and stability for the chemical environment like pH, polarity. BODIPY-derivatives have been synthesized to control the photophysical properties. Here, we revisited the photophysical properties of the BODIPY compound: Pyrromethene 546 which has the five methyl branches in the original BODIPY structure. In this study, when changing the concentration of BODIPY from 1 μM to 4 mM, we found that absorption and excitation spectra were significantly changed although the emission spectrum was almost the same. In the spectra at the different concentrations, we found that there were five different absorption bands. Two bands were red-shifted and the other two bands were blue-shifted when increasing the concentration. Interestingly, the emission spectrum from these five bands was the same and their lifetime was very similar (~ 8 ns).

Poster Presentation : **PHYS.P-100**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Linker Effects on Phase Separation Propensity of Multi-Domain Protein

Da-Eun Hwang, Jeong-Mo Choi[*]

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. Two types of proteins are known to drive phase separation: multi-domain proteins and intrinsically disordered proteins. 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. However, it is not clear how the properties of the linkers affect the LLPS propensity. We designed a new multi-domain protein system that can induce phase separation, by employing well-known fluorescent proteins as building blocks. Using this system, we studied the linker effects on LLPS by simulation and experiment. We found that a short linker leads to “shielding” of the binding interfaces on the folded domains, which results in the reduction of the LLPS propensity, and that if a linker is sufficiently long, the details of the linker (*e.g.* flexibility) become relatively less important.

Poster Presentation : **PHYS.P-101**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Structures of o-Toluidine-Water (oTW$_n$) Cluster Cation (n<=3)

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

Department of Chemistry, Kyung Hee University, Korea

The cluster ions are the center of the science of chemistry and biology. Especially, aniline derivative clusters have significant properties such as hydrogen bonding therefore it is essential to study their characteristics. Here, size-selective o-toluidine which is known as methyl aniline cluster cation was investigated using infrared action dissociation spectroscopy. This observation was focused on the 2800 ~ 3800 cm-1 range since NH and OH stretching were the important functional groups that indicated structures for clusters. These results were compared by theoretical data that was calculated by Gaussian 16 programs. The optimized structures and frequencies were performed by a combination of density functional theory and basis set (B3LYP/cc-pVQZ).

Poster Presentation : **PHYS.P-102**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Investigation of the Effect of the Form of Hafnium Zirconium Oxide ($Hf_{0.6}Zr_{0.4}O_2$) Co-Catalyst on the Photoelectrochemical Water Oxidation Efficiency of Hematite (α-Fe_2O_3)Photoanode

Hee Won Kim, Woon Yong Sohn[*]

Department of Chemistry, Chungbuk National University, Korea

We fabricated the hematite (α-Fe_2O_3) photoanode with $Hf_{0.6}Zr_{0.4}O_2$ (HZO) based co-catalysts prepared by two different types of the surface treatments, the overlayer coating and the deposition of the nanoparticles, to understand the effect of the form of the co-catalysts on the photoelectrochemical (PEC) performance. When the HZO nanoparticles were deposited on the surface of the hematite photoanode, the photocurrent density at $1.23V_{RHE}$ was 0.15 mA/cm^{-2}, which was improved by about 11%, compared to that of the bare hematite film. On the other hand, in the case of the HZO overlayer, the photocurrent density drastically decreased. (0.038 mA/cm^{-2} at $1.23V_{RHE}$). In this study, we successfully revealed using one of the time-resolved spectroscopic techniques, heterodyne transient grating (HD-TG) technique, and photo-electrochemical impedance spectroscopy (PEIS), that HZO nanoparticles could act as a cocatalyst, resulting in the enhancement of the charge transfer efficiency of the surface trapped holes, while the overlayer treatment did not influence the hole transfer kinetics and rather promoted the surface recombination.

Poster Presentation : **PHYS.P-103**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Calculation of dielectric constant of polymers using DFTB-MD and DFT method

Kihwan Yoon, Hyuna Shin, Dakyeung Oh, Joonghan Kim[*]

Department of Chemistry, The Catholic University of Korea, Korea

We developed a protocol to calculate a dielectric constant of polymers. We used a formula that contains fluctuation of total dipole moment to calculate the dielectric constant. Molecular dynamics (MD) simulations based on density functional tight-binding (DFTB) were performed, and single-point energy calculations using density functional theory (DFT) were performed on the trajectory generated by DFTB-MD. The dipole moments of polymers were calculated quantum mechanically and semi-classically. Various MD simulation parameters such as simulation time, size of the model, and volume were tested, and their effect on the calculation of the dielectric constant are discussed.

Poster Presentation : **PHYS.P-104**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Z-scheme $W_{18}O_{49}/ZnIn_2S_4$ Nanohybrid Catalyst for Enhanced Photocatalytic CO_2 Reduction

Jehee Lee, Tae Kyu Kim*

Department of Chemistry, Yonsei University, Korea

The conversion of CO_2 to hydrocarbon fuels through solar-driven energy has been proposed as a promising strategy to overcome the environmental problems, such as high CO_2 emissions and energy crisis. Among a variety of materials that have been investigated for photocatalysts in the production of fossil fuels from CO_2 in water, we suggest $W_{18}O_{49}$ and $ZnIn_2S_4$ for greatly accelerate the charge carrier separation and electron transport in the catalytic system. $W_{18}O_{49}/ZnIn_2S_4$ Z-scheme heterojunction photocatalyst was successfully synthesized via an in-situ method and applied to visible-light photocatalytic CO_2 reduction. Under illumination of visible light, the CO production rates over optimized $W_{18}O_{49}/ZnIn_2S_4$ photocatalyst was 9.8213 mmol g^{-1} h^{-1}, which was 1.52 times higher than that of pristine $ZnIn_2S_4$. In this case, Co complexes: $[Co(bpy)_3]^{2+}$ (bpy=2,2'-bipyridine) was used as an electron mediator to improve electron delivery to CO_2. Moreover, $W_{18}O_{49}/ZnIn_2S_4$ had a morphology that $W_{18}O_{49}$ nanowires were wrapped with $ZnIn_2S_4$ nanosheets. Herein, specific morphologies and Z-scheme mechanisms of photocatalysts are discussed, and perspectives in this inspiring area are also provided.

Poster Presentation : **PHYS.P-105**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Attainability of planar tetracoordinate fluorine atoms in FIn4+, FTl4+, FGaIn3+, FIn2Tl2+, FIn3Tl+, and FInTl3+.

Dakyeung Oh, Hyuna Shin, Kihwan Yoon, Joonghan Kim*

Department of Chemistry, The Catholic University of Korea, Korea

Recently, a theoretical investigation proposed six cations (FIn4+, FTl4+, FGaIn3+, FIn2Tl2+, FIn3Tl+, and FInTl3+) that contain planar tetracoordinate F (ptF) atom based on the density functional theory (DFT) and coupled-cluster singles and doubles with perturbative triples (CCSD(T)) calculations. We concluded that ptF atoms could not exist up to date based on CCSD(T) with very large-sized basis sets. The actual minimum structures of six cations are not planar structures but three-dimensional structures. The origin of distortion from the planar structures may be pseudo-Jahn-Teller distortion. We discussed this possibility.

Poster Presentation : **PHYS.P-106**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Adsorption and bulk diffusion of hydrogen on electrochemically-fabricated ZnO nanowires of various diameters

Sher Ali Khan, Chang Min Kim[1,*]

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

Metal oxide Nanowires have wide variety of applications in modern technology and researches such as catalysis, electronic devices, gas sensors, and energy storage materials. The ZnO nanowire is a promising candidate for chemical and biological nano sensors, but hydrogen impurities greatly effect the electrochemical properties of ZnO nanostructures. It is quite important to understand the incorporation of hydrogen in the bulk of ZnO. In this presentation, we will report the fabrication of ZnO nanowires and the diffusion of hydrogen into the bulk. ZnO nanowires of different diameters have been fabricated electrochemically by sol-gel method using anodized aluminum oxide (AAO) templates. Their morphological and structural properties were analyzed by atomic force microscopy (AFM), field emission scanning electron microscopy (FE-SEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The adsorption and bulk diffusion of hydrogen on ZnO has been studied using a temperature programmed desorption (TPD) method in ultrahigh vacuum (UHV).

Poster Presentation : **PHYS.P-107**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Inductive effects of ortho-Trifluoromethyl Substituent on Benzoyl Chloride in Solvolysis Mechanisms

Seoyeon Jang, YongGun Kim[1], Kyoung-Ho Park[2,*], Hoshik Won[1], Jin Burm Kyong[1], Dennis N. Kevill[3,*]

Applied chemistry, Hanyang University, Korea
[1]Department of Applied Chemistry, Hanyang University, Korea
[2]Department of Chemical Molecular Engineering, Hanyang University ERICA, Korea
[3]Chemistry & Biochemistry , Northern Illinois University , United States

The 2-(trifluoromethyl)benzoyl chloride was studied with the measurement of rates by conductivity skills and analyzed by the application of the Grunwald-Winstein(G-W) equations, activation parameters, the kinetic solvents isotope effect (KSIE), and the basic quantum mechanical calculations. The 2-(trifluoromethyl)benzoyl chloride has one of the very strong electrophilic substituent, trifluoromethyl group, at *ortho*-position. This substituent group has the inductive effect to withdrawal the π electrons on the benzene ring, and it could be respected to decrease the electron density on the reaction center of carbonyl carbon. The bond strength of between carbonyl carbon and chlorine is stronger than normal status, consequently. This factor could decrease the S_N1 character, and the *ortho*-position of substituent could be, also, the factor to decrease the S_N1 character sterically. The 2-(trifluoromethyl)benzoyl chloride has dual mechanisms that the addition-elimination is governed in the nucleophilic solvents except some deviated points and the dissociative S_N2 is governed in all electrophilic solvents by G-W equations. The activation parameters were resulted that $\Delta H^{\neq}$ = 12.6 ~ 13.8 kcal/mol and $\Delta S^{\neq}$ = -29.5 ~ -25.2 cal/mol·K in 100%EtOH(ethanol), 80%EtOH, and 100%MeOH(methanol), and that $\Delta H^{\neq}$ = 18.8 kcal/mol and $\Delta S^{\neq}$ = -8.3 cal/mol·K in 70%TFE(2,2,2-trifluoroethanol), respectively. These results are consistent with one of G-W equation analysis. The KSIE in 100%MeOH is reported 1.74 similarly.

Poster Presentation : **PHYS.P-108**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Ligand Chain Length Determines the Charge Transport and Energy Transfer Efficiency in InP/ZnSe/ZnS Quantum Dots

Jumi Park, Dongho Kim[1,*]

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

Non-toxic InP quantum dots (QDs) are promising light emitters for QD-based light-emitting diodes. Although the state-of-the-art InP QDs show high efficient, stable, and color purity photoluminescence (PL), it has been challenging to retain these excellent luminescent properties in electroluminescence (EL). Auger recombination, charge injection efficiency, or charge carrier mobility mainly govern the external quantum efficiencies (EQEs) of the QD light-emitting diodes (QLEDs). The organic capping ligands of QDs have been used to passivate the QD surfaces. However, it was reported that replacing surface ligands controlled the charge carrier mobility, charge injection, and balance in the spatial distribution of electrons and holes. Here we exploited the electrochemical charging method and revealed the effect of ligand chain length on the charge injection efficiency. Shortening the aliphatic ligand chain facilitated charge injection due to smaller barrier energy for charge transport. Further, we elucidated other factors in which organic ligands decide the luminescent efficiency of QD films. When the inter-dot distances are equal in QD superlattices, the aliphatic ligand chain length determines an energy transfer efficiency between neighboring QDs. We varied surface ligands and fabricated QD superlattices in InP/ZnSe/ZnS QDs. The Förster resonance energy transfer efficiency (FRET) is evaluated by fluorescence lifetime-intensity imaging (FLIM). The FRET dynamics is suppressed in QDs capped by ligands with a shorter aliphatic chain.

Poster Presentation : **PHYS.P-109**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Solid-to-Solid Transition of Organic Ionic Plastic Crystal under Shear

Chung Bin Park, **Bong June Sung**[*]

Department of Chemistry, Sogang University, Korea

Organic ionic plastic crystal (OIPC) is a unique class of a crystal in which orientational disorder is allowed while a long range translational order is maintained. Thanks to the rotational disorder, OIPCs have multiple solid phases with solid-solid transitions and undergo plastic deformations upon mechanical deformations. In this work, we show by employing atomistic molecular dynamics simulations that shear facilitates a solid-solid transition and produces unique plastic response. We employ 1,3-dimethyl imidazolium hexafluorophosphate ([MMIM][PF_6]) crystal and the step strain method to investigate mechanical response of the crystal. From our results, at low temperature and strain, [MMIM][PF_6] responses to a shear deformation like either elastic or viscoelastic solid. That is, with a step strain deformation, the crystal structure does not change or only a fracture can occur such that the stress does not decay (elastic solid) from the initial stress or converges to a smaller positive value (viscoelastic solid). On the other hand, at high temperature and strain, [MMIM][PF_6] changes its structure to a new crystal structure via spontaneous crystal-crystal transition. During the transition, ions rearrange their positions cooperatively and the stress relaxes to negative value which is not expected in the elastic or viscoelastic solid. Due to the transition, cations and anions are packed up layer by layer with a hexagonal structure. In the new crystal structure, ions obtain higher degrees of rotational disorder, which implies the increase of the rotational entropy. We find that shear can induce the solid-solid transition to increase rotational entropy and produce unique mechanical response different from the elastic or viscoelastic solid.

Poster Presentation : **PHYS.P-110**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Influence of Defects on the Dynamics and the Coordination Structure of Li^+ Ion in Organic Ionic Plastic Crystals

Hyungshick Park, Bong June Sung[*]

Department of Chemistry, Sogang University, Korea

Organic ionic plastic crystal (OIPC) is a class of solid electrolyte materials. In OIPCs, the interactions between ions are strong enough to form translationally ordered structure while the interactions are still weak enough to allow the rotational motions of ions. Due to this unique characteristic, dopant ions such as Li^+ can show fast ion dynamics and OIPCs can be utilized as solid electrolytes. Various ion transport mechanisms related to defects and grain boundaries. However, the length and lifetime scales of vacancies are too short to investigate via experimental techniques. Hence, the dominant ion transport mechanism in OIPCs is still in debate. In this work, we perform molecular dynamics simulations to understand the transport mechanism of Li^+ at a molecular level. We employ two kinds of defects: 1) a point defect and 2) a quasi-grain boundary. We calculate coordination numbers and mean squared displacements (MSDs) of Li^+. In the presence of point defects, Li^+ is coordinated with four anions, while the coordination number of a Li^+ is approximately three with no vacancies. The increase in the number of coordinated anions makes Li^+ hard to diffuse, thus decreasing the MSD of Li^+ compared to vacancy-free condition. On the other hands, the dynamics of Li^+ shows opposite trends with quasi-grain boundary. Diffusivity of Li^+ becomes faster with quasi-grain boundaries. This indicates that consecutive dislocations of ions at grain-boundary accelerate the diffusion of Li^+ despite of higher coordination number compared to defect-free condition. In the future work, we will test the universality of these trends in other OIPC families such as phosphonium base OIPCs.

Poster Presentation : **PHYS.P-111**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Reversibly photo-switchable hydrogel for re-writable device and drug delivery

Eunchae Kim, Namdoo Kim[*]

Division of Chemistry, Kongju National University, Korea

Eunchae Kim and Namdoo KimDepartment of Chemistry, Kongju National University, Gongju 32588, Republic of KoreaHydrogel is a cross linked water-inflatable polymer. It is used as a useful biomaterial in the drug delivery and tissue engineering fields because it has similar physical properties with bio tissues. Here, we introduce synthesis of a new hydrogel that could be tuned its own physical state spatiotemporally using pdDronpa (photo-dissociable dimeric Dronpa) which is a green fluorescent protein reversibly responds to the specific wavelengths. The synthesized hydrogel was photo-switchable under cyan light and violet light that could be used to make a re-writable device using photomasks. Finally, we made DNA-containing hydrogels to release DNA fragments by cyan light illumination to demonstrate that the light controllable hydrogels can be applied to drug delivery.

Poster Presentation : **PHYS.P-112**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Substituents Effects of Corrole Derivatives to Generate Singlet Oxygen

<u>Jun Yong Shin</u>, Won-Sik Han[1,*], Kang-Kyun Wang[2,*]

Research Center, BI Bio-photonics Co., Ltd., Korea
[1]*Department of Chemistry, Seoul Women's University, Korea*
[2]*BI bio-photonics Co., Ltd., Korea*

The physical, chemical, and biological properties of singlet oxygen have been received much attention. In particular, photosensitized oxidations involving singlet oxygen are implicated in photodynamic inactivation of viruses and cells, in phototherapy of cancer, and in photocarcinogenesis. In this work, a series of corrole derivatives, PC, PFPC, and MCPC, were investigated to study the correlation between the molecular structures and singlet oxygen generation efficiency. To investigate structure-property relationship, photophysical and electrochemical properties of three compounds were systematically investigated along with DFT calculations. Depending on the substituent, their quantum yield of singlet oxygen were varied.

Poster Presentation : **PHYS.P-113**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

The Inter-Domain Exchange and the Flip-Flop of Cholesterol in Tertiary Component Lipid Membranes and their Effects on Heterogeneous Cholesterol Diffusion

Eun sub Song, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Cell membranes are heterogeneous with a variety of lipids, cholesterol and proteins, and are composed of domains of different compositions. Such heterogeneous environments make the transport of cholesterol complicated: cholesterol not only diffuses within a particular domain but also travels between domains. Also, it flip-flops between upper and lower leaflets such that cholesterol may reside both within leaflets and in the membrane center between two leaflets. How the presence of multiple domains and the inter-domain exchange of cholesterol would affect the cholesterol transport, however, remains elusive. In this study, we perform molecular dynamics simulations for ternary membranes, which consist of saturated lipids (DPPC), unsaturated lipids (DIPC) and cholesterol. The ternary membranes in our simulations form two domains readily: DPPC and DIPC domains. Cholesterol prefers the DPPC domain to the DIPC domain for all compositions of lipids and cholesterol in our study. Cholesterol diffuses much faster in the DIPC domain than in the DPPC domain and the flip-flop also does, which indicates that more cholesterol in DIPC domain reside in the membrane center. The mechanism of the inter-domain exchange differs for different domains: cholesterol tends to exit the DIPC domain through the membrane center for transition while it exits the DPPC domain through the leaflet for transition. Also, the kinetics for the DPPC-to-DIPC transition is up to 7.9 times slower than the DIPC-to-DPPC transition. Consequently, the lateral diffusion of cholesterol becomes significantly heterogeneous as a combined result of the flip-flop and the inter-domain exchange.

Poster Presentation : **PHYS.P-114**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Transient Reflectance Setup for Exciton Dynamics in 2D Molecular Crystals

Myeong in Song, Sunmin Ryu[*]

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

Understanding exciton dynamics in low-dimensional materials bears significant importance in photosynthesis, photocatalysis and photovoltaics. 2D molecular crystals are an ideal model system to study excitonic behaviors under extreme confinement. In this work, we report on a confocal transient absorption spectroscopy setup optimized for 2D inorganic and organic semiconductors. For a higher sensitivity and flexibility on sample requirements, the change in absorption was obtained in the reflectance mode. The reflectance of 100-fs probe pulses (660 ~ 1320 nm) was measured as a function of the time delay with respect to 140-fs pump pulses (520 nm) that was modulated at either 10 kHz or 20 MHz. The instrument response function determined by sum frequency generation was ~350 fs, mostly limited by the microscope objective. For monolayer MoS2 supported on 285 nm SiO2/Si substrates, transient reflectance signals at 660 nm showed a biexponential decay with lifetimes of 0.44 and 2.72 ps, which respectively originate from exciton formation and trapping by defects. Preliminary data on 2D PTCDA (perylenetetracarboxylic dianhydride) crystals will also be presented with future instrumentation plans.

Poster Presentation : **PHYS.P-115**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Study of poly(alkylene carbonate) based solid polymer electrolytes using FTIR and 2DIR spectroscopies

Seoeun Shin, **Chaiho Lim**, **Kyungwon Kwak**[*], **Minhaeng Cho**[*]

Department of Chemistry, Korea University, Korea

In the last few decades, polyethylene oxide (PEO) based solid polymer electrolytes (SPEs) have been attracted because of high solvation power of PEO, good mechanical properties, and improved safety towards to conventional liquid electrolytes. However, low ionic conductivities of conventional PEO based SPEs are one of major problem of SPEs. Moreover, narrow electrochemical window of PEO also limits further applications of PEO based SPEs. To overcome these drawbacks, many researchers have tried to make SPEs with other polymers and several polymers including polycarbonates show higher performances than PEO. Among those polymers, we focused on polyethylene carbonate (PEC) and polypropylene carbonate (PPC) because they have carbonyl groups which are sensitive to changes of surroundings. In this study, we investigated PEC and PPC based SPEs with FTIR and 2DIR spectroscopies and acquired structural and dynamics information about those SPEs.

Poster Presentation : **PHYS.P-116**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Revealing the Reaction Mechanism of Nickel-Catalyzed Cross-Coupling Reaction by Using Time-Resolved X-ray Absorption Spectroscopy

Yeseul Han, Sangmin Jeong, Kyung Hwan Kim*

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

Carbon-oxygen cross coupling reaction with nickel catalyst is one of the most intense research subjects. They are uncommon since the essential step for the reaction (the reductive elimination of the Ni^{II} intermediate) is known to be unfavorable. Introducing photo-excitation can be a solution to the difficulty, but its mechanism is ambiguous. With Ir photocatalyst, the excited photocatalyst could activate the Ni^{II} intermediate by excitation or a redox reaction (1-2). Also, the direct excitation mechanism has been proposed in which excited Ni causes the reaction itself through aryl homolysis (3). Even though these mechanisms have been suggested and under fierce debate, there is no direct experimental evidence to point which mechanism is correct since it is hard to distinguish the Ir photocatalyst and the Ni intermediates in the UV-visible region (4). In this work, we predict the XANES spectrum of the Ni intermediate using theoretical calculation and demonstrate the feasibility of the XANES experiment distinguishing the Ni intermediates having different oxidation states. With extremely intense X-ray sources, such as an X-ray free electron laser, the TR-XANES technique will be the advantageous approach to explain the reaction mechanism of the Ni catalyst.Reference[1] E. R. Welin *et al*., *Science* **2017**, 355, 380-385[2] R. Sun, Y. Qin, D. G. Nocera, *Angew. Chem. Int. Ed.* **2020**, 59, 9527-9533[3] S. I. Ting *et al.*, *J. Am. Chem. Soc.* **2020**, 142, 5800-5810[4] L. Tian *et al.*, *J. Am. Chem. Soc.* **2020**, 142, 4555-4559

Poster Presentation : **PHYS.P-117**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

The Effect of Relative Flexibility of a Single Ring Chain in Linear Polymer Films on Its Spatial Arrangement and the Diffusion

Jong Ho Choi, Bong June Sung*

Department of Chemistry, Sogang University, Korea

The flexibility of a polymer chain determines its conformation and transport properties, and is considered to be an intrinsic property of the polymer. In polymer blends, not only the flexibility of each chain but also the relative flexibility difference would affect the properties of polymers. We conduct molecular dynamics simulations for a single ring polymer chain in thin films of linear polymer melts to show that the relative¬¬ flexibility of the ring chain (compared to the flexibility of linear chains) determines its location within the films and lateral diffusion. We tune the flexibility of ring and linear chains by changing the bending angle potential parameters while other intra- and inter-molecular interaction potentials are identical for both ring and linear chains. We find that it is not the flexibility of individual polymer chains but the relative flexibility that determines the spatial arrangement of the ring chain in thin polymer films. When a ring polymer chain is more flexible (more rigid) than linear polymer chains, the ring polymer is more likely to be located at the film surface (the film center). We find that such spatial arrangement should originate from the conformational entropy of the chain. The ring chain at the film surface (at which the local mobility is higher than at the film center) becomes flat such that linear chains penetrate the ring chain less and the ring chain may diffuse faster. Therefore, the relative flexibility determines not only the spatial arrangement but also the lateral diffusion of the ring chain.

Poster Presentation : **PHYS.P-118**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Revealing the structure of I atom - benzene charge transfer complex by time-resolved X-ray solution scattering

Seonju You, Kyung Hwan Kim*

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

In radical alkane halogenation, a fundamentally important process for synthesizing alkyl halides, the solvent effects are found to be critical in controlling the selectivity of halogen radicals reacting with substituted alkanes. In 1955, Russell and Brown discovered that benzene and other aromatic hydrocarbons, when used as a solvent, improve the selectivity of Cl radical to react with the tertiary carbon over the primary carbon in photochlorination of a substituted alkane, 2,3-dimethylbutane (DMB). According to this result, Russell initially proposed that the Cl radical and benzene could form an η^6-π complex. This π-complex is proposed to reduce the highly reactive nature of Cl radical and react more selective toward the chlorination of tertiary carbon than the primary carbon. However, the π-complex proposed by Russell and Brown was questioned. Skell and co-worker proposed an alternative species, a σ-complex based on the observation of a different reaction profiles in their experimental condition. In addition, a recent DFT calculations expects that the η^1-arene and Cl radical interaction would be the most stable among possible coordination geometries between benzene and Cl radical. Due to the lack of further conclusive spectroscopic evidence, the structure of halogen atom – aromatic charge transfer complex remains controversial and elusive.Our experiment aims to elucidate the structure of I atom - benzene complexes by time-resolved X-ray solution scattering. Using the various candidate molecular structure, we calculated the expected difference scattering intensities. Each structure candidate exhibits a unique curve pattern that will allow us to study the structural changes accompanying the photodissociation.

Poster Presentation : **PHYS.P-119**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

$CsCu_xPb_{1-x}Br_3@SiO_x$ Core-shell Perovskite Quantum Dots: Development of Synthetic Strategy under Ambient Condition at Room Temperature and their Cu Doping Induced Photophysical Properties.

Sumi Seo, Soo Jeong Lee, YouJeong Lee, Seog Joon Yoon[1,*]

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

ABX_3 perovskites have been numerously studied to various fields such as ferroelectronics, actuators, sensors, and current solar driven chemistry. In early 21st century, the organometal lead halide perovskites were vastly used to solar cells by enhancing their performances up to 25.2%. Also, varying the multi-dimensional perovskite opens more versatile applications to photocatalysis, CO_2 reduction, quantum dot light emitting diodes, *etc.,*. To commercialize the various perovskites, decreasing energy payback time, increasing performances of the perovskite-based devices, enhanced stability against H_2O and O_2, and decreasing the toxic elements are quite necessary. We developed synthetic strategy to do substitution of toxic Pb in the core-shell perovskites to Cu and its effect to the material and photophysical properties.

Poster Presentation : **PHYS.P-120**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Adsorption structures of organic molecules with propyl moiety containing different electronegative atom on Ge(100)

Jeong-Woo Nam, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

We investigated the adsorption structures and mechanisms of 1-propanethiol, 1-propanol, and 1-propylamine molecules containing S, O, or N atom on a Ge(100) surface. Through the analysis of high-resolution photoemission spectroscopy (HRPES) experimental data, 1-propanethiol and 1-propanol molecules showed dissociative adsorption behavior on the Ge(100) surface, whereas 1-propylamine exhibited N dative adsorption behavior at 0.3 Langmuir coverage. In addition, the adsorption behaviors confirmed by HRPES were supported by the reasonable transition energies and structures on the basis of density functional theory (DFT) calculations. These results for organic molecules with propyl moiety containing different electronegative atom adsorbed on the Ge(100) surface provide systematic information that expands current knowledge about the surface reactions of aliphatic molecules with alkyl chains.

Poster Presentation : **PHYS.P-121**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Translational Normal Mode Decoupling of Poly(ethylene oxide) melts; Breakdown of Time-Temperature Superposition

Hye Sol Kim, Bong June Sung[1,*]

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

The elastic moduli of linear viscoelastic materials can be estimated at a wide range of temperatures by superimposing the elastic moduli of different time scales at one reference temperature. This is known as the time-temperature superposition (TTS) principle, which assumes that the relaxations of all modes of polymers would have the same temperature dependence. Unfortunately, TTS sometimes breaks down, especially when the temperature near the glass transition temperature (T_g), of which origin remains a matter of debate. In this work, we investigate the spatially heterogeneous dynamics, which emerges near the glass transition, would be responsible for the TTS breakdown. We employ OPLS-AA force field and perform all-atom molecular dynamics simulations for poly(ethylene oxide) (PEO), which have taken center stage for the next generation solid polymer electrolytes. We calculate the dynamic structure factor F_i (k,t) (which is the Fourier-transform of the space-time correlation function of a polymer segment) for several segmental modes of PEOs. Here, *i*, *k*, and *t* denote the index of each segmental mode, a wave vector and time, respectively. We estimate the friction coefficient (ζ_i) of the *i* th segmental mode by fitting F_i (k,t) to a Kohlrausch-Williams-Watts (KWW) stretched exponential function. We find that as temperature decreases down to the glass transition temperature, the segmental dynamics becomes heterogeneous such that the ratios of ζ_i's decouple to one another and ζ_i's do not show identical temperature dependence, which is against the underlying assumption of TTS principle.

Poster Presentation : **PHYS.P-122**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

The Translation-Rotation Decoupling of Tracers Reflects Medium-Range Crystalline Order in Two Dimensional Colloid Glasses

Dong jae Chun, Bong June Sung[1,*]

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

In glasses and supercooled liquids, the dynamics becomes extremely slow and spatially heterogeneous. One of their complex dynamic signatures is the translation-rotation decoupling, which means that D_T/D_R does not stay constant over a range of temperature anymore. Whether and how the dynamic heterogeneity and the translation-rotation decoupling would relate to local structure of glasses has been a puzzle for decades. In this work, we perform molecular dynamics simulations for both two dimensional polydisperse colloids (2DPC) and two dimensional binary colloids (2DBC) with tracers. In 2DPC glasses, hexatic local structures, which is well-known as the medium-range crystalline order (MRCO), develop at low enough temperature and grow quickly along with the dynamic correlation length. In 2DBC glasses, on the other hand, any explicit local structure has not been reported to grow with the dynamic correlation length at low temperatures. Here, we employ two different types of tracers: a diamond tracer that resembles the MRCO of 2DPC glasses and a square tracer that is dissimilar to any local structure of glasses. We show that the translation-rotation decoupling of the diamond tracer is much more significant than that of the square tracer in 2DPC glasses. On the other hand, such a shape-dependence of the decoupling is not observed in 2DBC. We introduce a shape-dependency parameter of the decoupling and find that the shape-dependency parameter grows along with the dynamic correlation length in 2DPC glasses but not in 2DBC glasses. This illustrates that the dynamic heterogeneity and the translation-rotation decoupling of tracers should reveal the local structures of glasses.

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Poster Presentation : **PHYS.P-123**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Generation of deeply supercooled water droplets for revealing a hypothetical fragile to strong transition of liquid water

MyeongSik Shin, Kyung Hwan Kim*

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

Most liquids can be classified into two categories, fragile and strong ones, depending on their temperature dependence of the dynamics. Water at ambient temperature and modest supercooled conditions is considered to be a fragile liquid whereas it is proposed to be a strong liquid at temperatures close to the glass transition, which is 135 K. However, it is postulated that there exists a fragile to strong transition somewhere in the deeply supercooled regime. By time-resolved Optical Kerr Effect (OKE) scattering and evaporative cooling in vacuum condition can give chance to find those properties. For the OKE scattering measurement on supercooled water at PAL-XFEL, we have built the equipment that can generate deeply supercooled water droplets and have successfully tested it down to ~227 K. References :[1]K. H. Kim et al., Science 358, 1589-1593 (2017).[2]J. A. Sellberg et al., Nature 510, 381-384 (2014)[3]R. Torre et al., Nature 428, 296-299 (2004)[4]A. Taschin et al., Nat. Commun. 4, 2401 (2013)

Poster Presentation : **PHYS.P-124**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Jet-cooled spectroscopy of the isomeric chloro-p-xylyl radicals in a coronaexcitedsupersonic expansion

Changsoon Huh[*], Jaehyuck Kim

Applied Chemistry, Dong-Eui University, Korea

Poster Presentation : **PHYS.P-125**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Full Three-Dimensional Non-Adiabatic Quantum Dynamics of The Bidirectional Proton-Coupled Electron-Transfer Process in FHCl System

Pinit Ariyageadsakul, Kyoung-Koo Baeck*

Department of Chemistry, Gangneung-Wonju National University, Korea

The early time dynamics of FHCl is a simplest but realistic system showing bidirectional proton-coupled electron transfer (PCET) process, i.e., the charge-transfer excited state F+H–Cl– proceeds to two dissociation paths generating F + HCl (proton transfer, PT) and FH + Cl (electron transfer, ET) products. The MRCI/aug-cc-pVTZ method was employed to evaluate the adiabatic potential energy surfaces (PESs) of low-lying electronic states in full three-dimensional spaces of FHCl, and the diabatic potential energy surfaces of coupled electronic states were constructed by using our own methods explained elsewhere [1,2,3]. The quantum mechanical behavior of nuclei were examined by solving the time dependent Schrödinger equation up to several hundreds of femtoseconds. Our results show that the PT process starts significantly faster than the ET process (20 fs vs. 100 fs), and the calculated branching ratio (PT/(PT + ET)) = 0.67 implies the dominance of PT process. The photoabsorption spectrum of FHCl was also simulated by Fourier transformation of autocorrelation function, and its dependence on the initial vibration level of precursor anion was examined to simulate actual results of future IR+UV two photon experiments. The vibration distribution of fragmented products was analyzed by calculating the overlap integral between the accumulated wave-packet absorbed by negative imaginary potential (NIP) at the dissociation limit and the vibrational wave function of the fragmented product molecule at several vibration states. Dependences of the above factors on isotope substitution of the connecting H atom were studied too.[1] H. An and K. K. Baeck, J. Chem. Phys. 143, 194102 (2015). [2] K. K. Baeck and H. An, J. Chem. Phys. 146, 064107 (2017).[3] P. Ariyageadsakul and K. K. Baeck, J. Chem. Phys. 154, 154305 (2021).

Poster Presentation : **PHYS.P-126**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Nf/PVP/rGO/$CuInS_2$ Hybrid Composite Photocathode for Efficient Photoelectrochemical CO_2 Reduction into Formaldehyde

Hyun Ho Jung, Young soo Kang[*]

Department of Chemistry, Sogang University, Korea

The optimized p-$CuInS_2$ (CIS) thin film as a pristine photocathode for CO_2 reduction was fabricated through chemical deposition method. The structural, optical and photoelectrochemical properties of CIS thin film were investigated. The maximum net photocurrent density of bare CIS thin film reached almost around 0.26 mA/cm^2 at - 0.5 VAg/AgCl, which is much higher value than that of the previously reported one. In order to improve the solar-to-fuel efficiency for CO_2 reduction, reduced graphene oxide (rGO) poly(4-vinyl)pyridine (PVP) and nafion (Nf) were coated on the surface of /CIS thin film step by step to have sequential multi electron shuttling, CO_2 adsorption and activation and one pot reaction of multiple proton-coupled electron transfer to CO_2 molecules, respectively. rGO and Nf have superior electron and proton conductivity, so it can facilitate the multiple proton-coupled electron transfer on the CIS electrode surface. The CO_2 reduction experiments were carried out using CIS, rGO/CIS, PVP/rGO/CIS and Nf/PVP/rGO/CIS photocathodes coupling with $BiVO_4$ photoanode, respectively, in the same PEC system and compared solar to fuel (STF) efficiencies of them comparatively. Formaldehyde was detected with gas chromatography (GC) as a solar fuel of produced hydrocarbon product with minor hydrogen gas bubbling and the production yield was gradually increased by coating rGO, PVP and Nf, subsequently. The improved STF efficiency was achieved to ca. 0.132 % by Nf/PVP/rGO/CIS electrode.

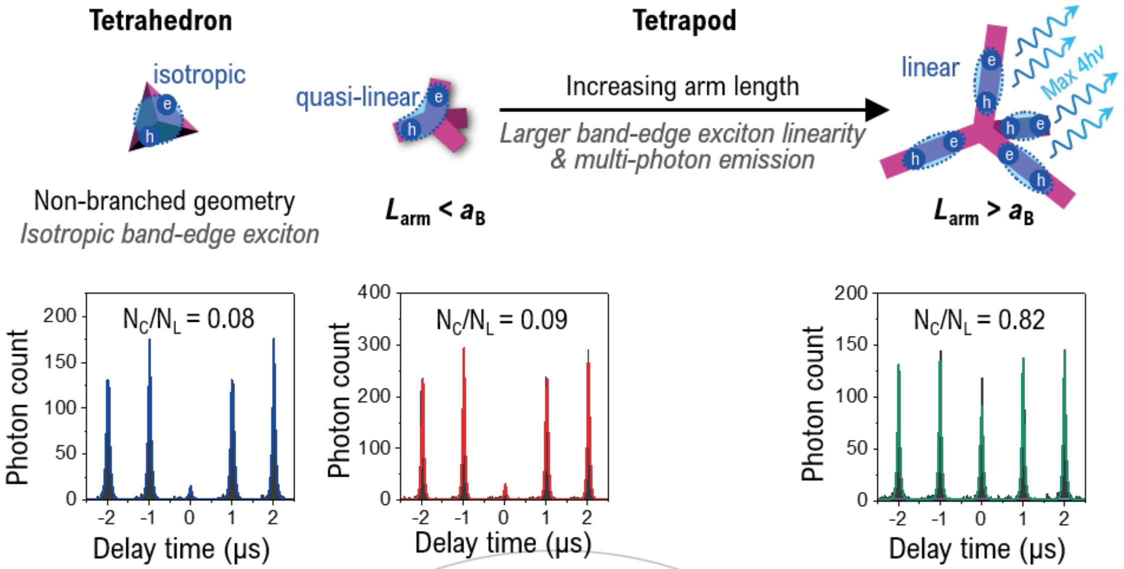
Poster Presentation : **PHYS.P-127**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Tailoring the functionality of single crystalline InP tetrapod nanocrystals

Taehee Kim, Youngsik Kim[1], Dongho Kim[*], Sohee Jeong[1,*]

Department of Chemistry, Yonsei University, Korea
[1]*Department of Energy Science, Sungkyunkwan University, Korea*

Semiconductor materials constitute the firm basis of modern lifestyle, in that their properties make possible the technological wonders ranging from hand-held electronics and to solar cells and fiber-optic communications. Property of a semiconductor material is conducted by the fate of its electron-hole pair (exciton); thus, manipulating exciton behavior has long been the primary objective of the nanomaterials field. In particular, nanocrystal particles exert strong spatial confinement that is in charge of their unusual excitonic characteristics. However, this confinement quickly vanishes the multiexciton species, making the interactions between nanocrystal excitons remain rarely studied, unless intentionally fabricated. Here, we present a novel platform for exciton engineering using a straightforward strategy of nanocrystal shape-tuning. Thanks to the unique branched geometry, single crystalline tetrapods demonstrated a transition from single to multi-photon emitter upon tetrapod arm length extension. This accompanied change in exciton confinement orientation from 3D to 2D-like confinement, which not only narrowed the distribution of single nanocrystal band gap energy but also enhanced the polarization response of material. Interactions among multiple excitons in long-armed tetrapod, which involve an increase in quantum-confined Stark effect, were found to promote the enhancement of memory effect in single nanocrystal blinking. Overall, these results provide an explicit vision for the future design strategy and synthetic control of functional nanomaterials for desired purposes.


Tetrahedron
isotropic
e
h
Non-branched geometry
Isotropic band-edge exciton
quasi-linear
$L_{arm} < a_B$
Tetrapod
Increasing arm length
Larger band-edge exciton linearity
& multi-photon emission
linear
Max 4hν
$L_{arm} > a_B$
$N_C/N_L = 0.08$
$N_C/N_L = 0.09$
$N_C/N_L = 0.82$
Photon count
Delay time (μs)
0
50
100
150
200
300
400
-2
-1
0
1
2

Poster Presentation : **PHYS.P-128**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Distribution Functions of Energy Barrier for Agglomeration of Magnetic Nanoparticles

Hackjin Kim

Department of Chemistry, Chungnam National University, Korea

Agglomeration of magnetic nanoparticles under the magnetic field is a typical example of complex process. The kinetics of the complex process is usually non-single exponential kinetics because the involved energy barrier is not the single value but has some distribution. The dynamics of the complex process corresponds to the Laplace transformation of the energy barrier distribution function. The inverse Laplace transformation of the observed dynamics results in the energy barrier distribution function while the analytical solution for the inverse Laplace transformation is not always available. The stretched exponential kinetics is observed in the agglomeration of magnetic nanoparticles under the magnetic field. The inverse Laplace transformation of the stretched exponential gives the analytical solutions only for some special cases. Interesting feature of the energy barrier distribution function from the stretched exponential kinetics is that the distribution function is negatively skewed. In this work, the physical meanings of the negatively skewed energy barrier spectrum are examined and, various energy spectra such as the Planck distribution function for the black-body radiation, the exponentially modified Gaussian distribution and some other functions are compared with the energy spectrum from the stretched exponential kinetics.

Poster Presentation : **PHYS.P-129**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Conformational stability of tetrahydrofuran revealed by IR resonant VUV-PI/MATI spectroscopy

Sung Man Park, Taeung Eom[1], Chan Ho Kwon[1,*]

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

We probed the conformational stability of tetrahydrofuran (THF), which indicates the twisted and bent conformations in the S_0 state but is still disputable. Furthermore, the quantum chemical calculations predicted that the twisted (C_2 symmetry) and bent (C_s symmetry) conformers of the S_0 state are separated by a small interconversion barrier, whereas only the twisted conformer exists in the D_0 state. It implies that identifying the contribution of each conformer in the S_0 state is immensely difficult because the VUV-MATI spectroscopy reveals only the ionic transitions of twisted conformer. Accordingly, we measured the IR absorption spectrum of THF utilizing the IR resonant VUV-PI scheme, which is contributed by both the twisted and the bent conformers. Then, the IR dip VUV-MATI spectrum of the twisted conformer was measured so as to be deconvoluted from the IR absorption spectrum of THF, which will unveil the contribution of the bent conformation in the IR absorption spectrum. To check the conformational stability, the deciphered IR absorption spectra corresponded to two conformers in THF were measured under various molecular beam conditions, which affect the relative populations of two conformers in the S_0 state.

Poster Presentation : **PHYS.P-130**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced Chemical Reactivity Induced by the Strong Coupling of Optical Cavity and a Molecular Vibration

Danbi Lee, Hankyul Lee, Zee Hwan Kim*

Department of Chemistry, Seoul National University, Korea

Vibrational Strong Coupling (VSC), the hybridization of molecular vibrational state and the Fabry- Pérot (FP) modes of the optical cavity surrounding the molecule, is known to alter the chemical reactivity. However, no clear molecular mechanism has not been established thus far. Here, we present systematic studies on VSC-induced reactivity changes in an attempt to gain molecular-level insight into VSC-induced chemistry of alcoholysis reactions under room temperature. The kinetic analysis of the infrared C=O stretching peak of the product reveals that the VSC enhances the reaction rates by three folds. Such reaction enhancement systematically increases for primary, secondary, and tertiary alcohols. We speculate that the enhanced reactivity mostly arises from the increase in the thermal population of vibro-polaritonic states of OH stretching mode. VSC has great potential in that it works in the dark and at room temperature, providing a way to approach selective chemistry.

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Poster Presentation : **PHYS.P-131**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Comprehensive computational study on the surface of oxygenated di-nickel di-selenide for hydrogen evolution reaction

Prabhakaran Sampath, Do hwan Kim[1,*]

Department of Nano Convergence Engineering, Jeonbuk National University, Korea

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

- Withdrawal -

Poster Presentation : **PHYS.P-132**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Solar fuel production via CO2 Reduction on the ZnO@ZnTe Photoelectrodes in a Photoelectrochemical System

Vaibhav Trivedi, Young soo Kang[1,*]

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

Carbon dioxide emission is increasing at an alarming rate which is very detrimental to the environment. It has a huge impact on the environment including the rising temperature and therefore, conversion of CO2 has been an area of interest for many researchers. It is necessary to convert CO2 into different useful products which can be used directly or as a feedstock for other products to complete the carbon cycle. Different catalytic methods, such as photocatalysis, electrocatalysis and photoelectrocatalysis have been reported to produce different fuel products such as methanol, ethanol, and methane. However, due to extremely stable structure of CO2 molecule, it is very difficult to convert it into its radical form. Huge amount of energy is required in the form of heat or electrons to overcome the reaction barrier. Different catalytic materials and their combinations have been used to overcome the energy barrier of CO2 conversion. In this work, photoelectrochemical (PEC) system was used for the CO2 conversion. BiVO4 photoanode was used to produce electrons and hole by photoinduced charge separation and protons by water splitting reaction in the anode compartment and CO2 reduction reaction takes place in the cathodic compartment on the surface of ZnO@ZnTe. Nanorod array film of zinc telluride coated on ZnO (ZO@ZT) provides large surface area rather than planar film and tunable range of reduction potential for CO2 reduction. Re-oxidation of CO2 reduction products by photo-generated holes on the surface of cathode was prevented by nafion between cathode and anode compartment. Functional layers such as reduced graphene oxide, polypyrrole and nafion were coated on the ZO@ZT electrode to enhance the performance of CO2 reduction reaction into liquid fuels. Different characterization techniques such as SEM, XRD, X-ray photoelectron spectroscopy (XPS), electrochemical techniques, GC, and GC-MS were used to confirm the formation of ZO@ZT photocathode and CO2 reduction reaction process. The whole system with the combination of photoanode and photocathode was used for the artificial photosynthesis and monitored water splitting and CO2 reduction rate.

Poster Presentation : **PHYS.P-133**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Photoelectrochemical Study of Copper Doped Hematite Thin Film

Young soo Kang*, Thomi Hawari[1]

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

In this study, the effects of Cu2+ ion doping into hematite thin film was been studied. X-ray diffractometer (XRD), scanning electron microscope (SEM), X-ray photoelectron spectroscopy (XPS) and Raman spectroscopy were used to observe alteration of hematite crystal structure after doping of Cu2+ ion. In XRD patterns, no observed peak shifting was occurring and XPS data confirmed that after doping with Cu2+ ion, the Fe/O ratio was increased as the dopant concentration increased. This alteration showed substitution of Fe3+ with Cu2+. In addition, Raman-inactive Eu mode was observed at 660 cm-1 in Raman spectrum after doping. The appearance of this mode might be related with defect formation due to substitution of Fe3+ with Cu2+. The resistivity of each sample was measured with electrochemical impedance spectroscopy (EIS). Comparing with the pristine hematite, the low amount of doping had smaller resistivity, but resistivity increased as the concentration of Cu2+ ion dopant increase. The Cu2+ ion present in the lattice caused distortion on the hematite crystal structure, which suppresses the electron transfer on the surface of the hematite thin film. Accordingly, the photocurrent density obtained with high concentration Cu2+ ion doped sample was decreased to 0.15 mA. On the other hand, lower concentration of Cu2+ ion dopant produced the highest photocurrent as 0.3 mA. In addition, the slope of Mott-Schottky plot was used to study the semiconductor properties of Cu2+ ion doped hematite thin film. As the concentration of Cu2+ ion dopant increased, the carrier density was decreased and the plot started to be reversed, which was shown by the alteration of properties from n-type semiconductor to p-type semiconductor. UV-vis diffuse reflectance spectra (UV-vis DRS) and UV photoelectron spectra was done to study the band formation of copper doped hematite thin film. The band gap of the samples was in 2.112 – 2.124 eV area and incident photon to current efficiency (IPCE) was showing the highest value of 4.6% at 0.23 V vs Ag/AgCl from 1 mol% Cu2+ doped hematite.

Poster Presentation : **PHYS.P-134**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

In Vitro Cellular Cytotoxicity and Relaxometric properties of Chitosan Oligosaccharide Lactate-coated Gadolinium Oxide Nanoparticles

Mohammad Yaseen Ahmad, **Gang Ho Lee**[1,*]

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

Chitosan oligosaccharide lactate (COL) has been modified to improve the water solubility of chitosan, especially for use in drug delivery and biomedical applications. The present study reveals that the suitability of COL as a surface-coating material of gadolinium oxide NPs is explored. COL-coated ultrasmall gadolinium oxide NPs were synthesized via a facile one-pot polyol method. The synthesized NPs (d_{avg} = 1.9 nm and a_{avg} = 19.5 nm) were nearly non-toxic, as evidenced by cellular cytotoxicity tests. They also exhibited good relaxometric properties (i.e., r_1 = 13.0 $s^{-1}mM^{-1}$ and r_2/r_1 = 2.1), confirming their suitability as a T_1 MRI contrast agent. This was further confirmed from the clear dose-dependent positive contrast enhancements in the R_1 map images

Poster Presentation : **PHYS.P-135**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Revealing the Reaction Mechanism of the Enyne Metathesis Reaction Catalyzed by the Grubbs Ru Complex

Sangmin Jeong, Seonju You, Kyung Hwan Kim*

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

Homogeneous transition metal catalyst is widely used in many research fields and industries. However, the detailed reaction mechanism is not well known since the intermediate species would only be populated for a short time and its overall concentration would be very low. One example is the enyne metathesis reaction with Grubbs Ru catalyst, which has a long-standing controversy on the reaction initiation step in ring-closing enyne metathesis and that is 'ene-first' vs. 'yne-first'. [1, 2] X-ray spectroscopy technique associated with ultrashort and bright X-ray beam from synchrotron/XFEL is very sensitive to the electronic structure of the metal complex and the type of surrounding ligands. [3] Thus, with the X-ray absorption spectroscopy associated with the stopped-flow technique, it is possible to study the reaction mechanism of the homogeneous transition metal catalyst by monitoring important but short-lived intermediates. Here, we studied the reaction mechanism of enyne metathesis reaction catalyzed by the Grubbs Ru complex to resolve a long-standing controversy for the two equally plausible reaction pathways. The XANES spectra of Grubbs Ru catalyst and its mixtures with alkene and alkyne substrates are obtained and compared with the theoretical spectra. By comparing the theoretical and experimental XANES spectra, we could conclude that there exist the difference peak shift in the ene-complex and the yne-complex. It implies the possibility of finding the true reaction mechanism of enyne metathesis reaction using the peak shift analysis in XANES spectra.[1] Lloyd-Jones, G. C. et al., Angew. Chem. Int. Ed., 44, 7442-7447 (2005)[2] Dieltiens, N. et al., Chem. Eur. J., 13, 203-214 (2007)[3] Cordones, A. A. et al., Nat. Commun., 9, 1989 (2018)

Poster Presentation : **PHYS.P-136**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Simple Synthesis of Side-by-Side Ag-AuNPs/Y 2 SiO 5 : Pr 3+ Up-conversionNanophosphors for Photochromic Applications

Hieu Minh Ngo, Young soo Kang[1,*]

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

Up-conversion phosphor material praseodymium-doped yttrium orthosilicate, Y 2 SiO 5 :Pr 3+ ,converts visible light into UV light (280 – 340 nm). However, this material has lowconversion efficiency, limiting its application. In this report, a side-by-side structureincluding up-converting phosphors combined with Ag NPs were developed, allowing theenhancement of the up-converting efficiency by using Ag NPs as light intensityamplification. Visible light intensity was enhanced by Ag NPs nearby, absorbed to the up-conversion material with higher efficiency. The materials were characterized primarily byTGA, XPS, TEM, EDS showing the clear side-by-side structure and underlying formationmechanism.

Poster Presentation : **PHYS.P-137**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Silica-Coated Core-Satellite Nanoassembly as a Stable, Sensitive, and Multiplex SERS Probe

Hoa Duc Trinh, Sangwoon Yoon[1,*]

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

Developing highly sensitive and stable surface-enhanced Raman scattering (SERS) probe systems is an actively pursued goal in sensors and diagnostics. In this study, we present silica-coated core-satellite ($CS@SiO_2$) nanoassembly structures that potentially realize this goal. We assemble Au nanoparticles (AuNPs) into core-satellite (CS) configurations using dithiol molecular linkers that also serve as SERS labels. Multiple hot spots in the CS structure and narrow nanogaps in each hot spot produce a significantly enhanced Raman scattering signal with an enhancement factor of ~6×10^7. Various types of molecules can be inserted into the nanogaps using the mixed self-assembled monolayers with alkanedithiol, enabling multiplex detection. Silica encapsulation of the CS particles stabilizes the particles and makes it easy to modify the surface to attach antibodies or DNAs. Many properties of the $CS@SiO_2$, including a wide range of optical resonances, scalability using multiple glass slides, long-term stability in ethanol, and single-particle-level sensitivity, make the material an ideal SERS probe for sensitive and multiplexed detection of diseases and viruses.

Poster Presentation : **PHYS.P-138**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

X-ray Attenuation Properties of Poly-(acrylic acid) and Poly-(acrylic acid-co-maleic acid)-coated Cerium Oxide CeO_2 Nanoparticles as a High-Performance CT Contrast Agent

Abdullah Al saidi, Gang Ho Lee[1,*]

Department of Chemistry, Kyungpook National University, Oman

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

Ultrasmall heavy metal-oxide has shown great potential as powerful X-ray attenuation coefficients. On other hand, it has been proven that X-ray attenuation depends on the x-ray source's voltage. Based on that, a synthesis different two polymers (poly(acrylic acid) (average M_w = ~1800 Da) and (PAA) Poly(acrylic acid-co-maleic acid) (PAAMA)(average M_w = ~3,000 Da))-coated cerium oxide nanoparticles using the height temperature polyol method. The synthesized nanoparticles exhibited excellent colloidal stability and biocompatibility with a nearly monodisperse particle diameter distribution, which was estimated to be 1.60 nm and 2.00 nm for PAA-CeO_2 and PAAMA-CeO_2 nanoparticles respectively from a lognormal function fit to obtain (d_{avg}). The plot of X-ray attenuation power (HU) as a function of the atomic concentration showed that the nanoparticle suspension samples' X-ray attenuation powers were strong. These findings indicate that the cerium oxide nanoparticle may be a potential CT contrast agent.

Poster Presentation : **PHYS.P-139**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Magnetic Properties, Water Proton Relaxivities, and Fluorescence Properties of D-Glucuronic Acid-Coated Ultrasmall Ln_2O_3 (Ln = Dy, Tb, and Ho) Nanoparticles

Dejun Zhao, Gang Ho Lee[1,*]

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

The lanthanide-based NPs are generally applied to magnetic resonance imaging (MRI), while some could also act as fluorescence imaging (FI) agents. Therefore, the obtained ultrasmall D-glucuronic acid-coated Ln_2O_3 (Ln = Dy, Tb, and Ho) NPs possess the average diameters of ~ 2 nm. All the samples showed appreciable magnetization (~ 4 emu/g) at the applied field (1.8 T) at room temperature, high transverse water proton relaxivities (r_2) of ~ 7s^{-1} mM^{-1} at 1.5 T, ~ 35 s^{-1} mM^{-1} at 3.0 T, and ~ 55 s^{-1} mM^{-1} at 9.4 T and negligible longitudinal water proton relaxivities (r_1), which could make them serve as T_2 MRI contrast agents at high applied field. Moreover, the obtained D-glucuronic acid-coated ultrasmall Tb_2O_3 NPs could also perform fluorescence in green region for dual-modal imaging.

Poster Presentation : **PHYS.P-140**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis and characterization of blue fluorescent carbon nanoparticles

Tirusew Tegafaw, Gang Ho Lee[*]

Department of Chemistry, Kyungpook National University, Korea

In this study, We report a simple one-step chemically synthesized fluorescent carbon nanoparticles in distilled water forming stable colloidal solution and non-toxic with ultra-small in size. The average particle size is 2.2 nm. Carbohydrates are used as a starting material to produce carbon nanoparticles. We studied the toxicity, optical and relaxometric properties of carbon nanoparticles. Under the irradiation of ultraviolet (UV)- visible absorption (λabs) at 267 nm and emission (λem) at 453 nm, the carbon nanoparticles show sky-blue in color. It can be suggested that carbon nanoparticles can be used as a T2 MRI contrast agent at a higher MR field.

Poster Presentation : **PHYS.P-141**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Ligand size and functional groups hydrophilicity effects on enhancement of Ho_2O_3 nanoparticles as T_2 MRI contrast agent

Shuwen Liu, Gang Ho Lee[1,*]

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

The relaxometric properties of ultrasmall Ho_2O_3 nanoparticles coated with various ligands were investigated. These ligands are named Poly (ethylene glycol) bis(carboxymethyl) ether (COOH-PEG-COOH) (Mn=250 and 600) with hydrophobic carboxyl groups, and large polyethylenimines (PEIs) with hydrophilic chains, namely, PEI-1300 and PEI-60000 (Mn= 1300 and 60000). From the research, the longitudinal (r_1) and transverse (r_2) water proton relaxivities generally decreased with increasing ligand-size (the ligand-size effect). Because the ligand layer thickness increased with increasing ligand size, which result in less water will access the nanoparticles. In addition, the diameter of nanoparticles were found to be ultrasmall and all samples were found to be non-toxic in cellular cytotoxicity tests.

Poster Presentation : **PHYS.P-142**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis, characterizations and applications of ultrasmall carbon coated Gd_2O_3 nanoparticles

Ying Liu, Gang Ho Lee[1,*]

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

In this study, a novel kind of carbon coated ultrasmall gadolinium oxide (Gd_2O_3@C) nanoparticles with paramagnetic gadolinium oxide core and luminescence carbon shell can be apply as contrast agents for both in vivo fluorescence imaging (FI) and magnetic resonance imaging (MRI). The nanoparticles were synthesized in aqueous solution by a facile method. The obtained Gd_2O_3@C NP with diameter of 3.1±1.0 nm exhibited not only high longitudinal relaxivity (r_1=16.26 s^{-1} mM^{-1} ; r_2/r_1 = 1.48) 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 shell. Therefore, this research revealed that the ultrasmall Gd_2O_3@C NPs suited for promising MRI and FI dual modal contrast agent to provide more accurate and comprehensive diagnosis information.

Poster Presentation : **PHYS.P-143**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Carbon-coated dysprosium oxide (Dy_2O_3@C) nanoparticles were synthesized as a new type of high-efficiency T_2 MRI contrast agent

Huan Yue, Gang Ho Lee[1,*]

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

Negative MRI contrast agents require high magnetic moments, nanoparticles can be considered as potential candidates for a new class of MRI contrast agents. Whereas, if nanoparticles can ignore the induction of longitudinal water proton spin relaxation, but can induce transverse water proton spin relaxation, they may provide negative contrast MR images even though their magnetic moments are not high, thus acting as an efficient T_2 MRI contrast agent. In this research, carbon-coated paramagnetic dysprosium oxide (Dy_2O_3@C) NPs (core = Dy_2O_3; shell = carbon) were synthesized and characterised to explore their potential as a T_2 MRI contrast agent for 3.0 T MR field. Due to an appreciable magnetic moment of the core Dy_2O_3 NPs which arises from fast 4f-electrons of Dy(III) (^{6}H15/2), the Dy_2O_3@C NPs exhibited an appreciable transverse water proton spin relaxivity (r_2) with negligible longitudinal water proton spin relaxivity (r_1). Therefore, as a highly efficient T_2 MRI contrast agent, there are negative contrast enhancements were observed in vivo T_2 MR images.

Poster Presentation : **PHYS.P-144**

Physical Chemistry

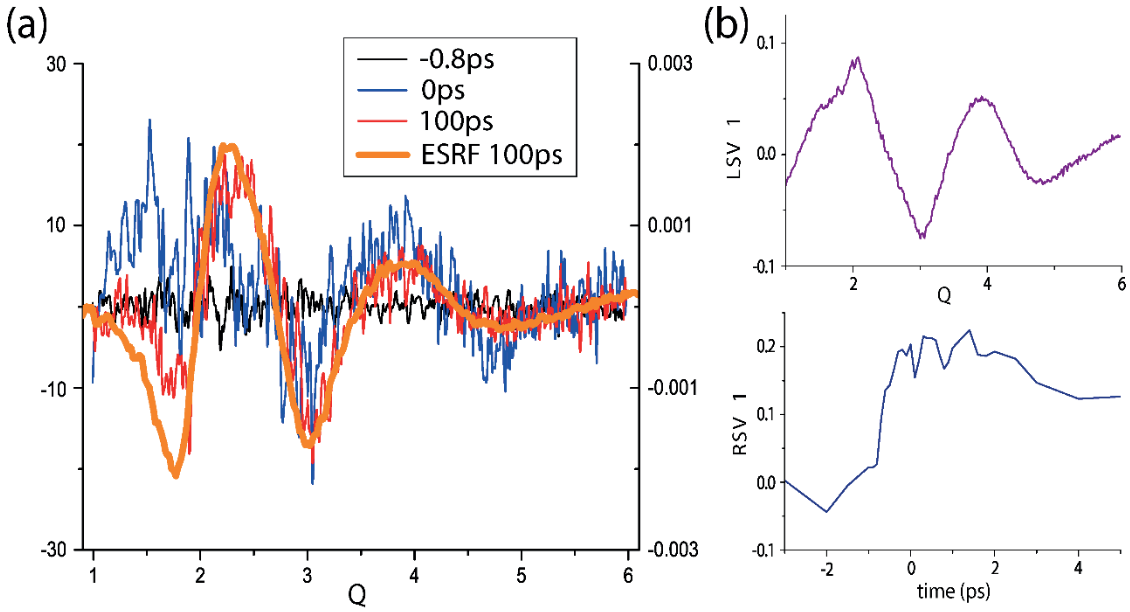
Exhibition Hall 1 THU 11:00~12:30

Effect of the enhanced solvent-solute interaction in the deeply supercooled regime on the structure of triiodide ion

Kyeongmin Nam, Seonju You, Kyung Hwan Kim*

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

Solvent-solute interaction is one of the key factors to comprehend various mechanisms and properties of the molecules. One such interaction is the hydrogen bonding interaction, which is common in an aqueous solution. Recent studies on I3- revealed that the hydrogen-bonding solvents make the solute have an asymmetric and bent structure due to the strong solvent-solute interaction. Since it is well known that the hydrogen bonding network gets stronger at supercooled temperatures, we have studied I3- in the supercooled solution to understand the effect of the enhanced solvent-solute interaction.[1] K. H. Kim et al., Phys. Rev. Lett. 110, 165505 (2013)[2] K. H. Kim et al., Science 358, 1589-1593 (2017)



Poster Presentation : **PHYS.P-145**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Aggregation of Hyperphosphorylated tau with Polyamines

Jinmin Lee, Sang Hak Lee[1,*]

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

In Alzheimer’s disease (AD), neuronal dementia was previously attributed to the accumulation of amyloid protein. However, many recent clinical studies targeting aggregation of amyloid have not shown any practical effect. Many studies have instead shown that protein is the major cause of dementia by creating neurofibrillary tangles (NFTs) in neurons. The neuronal tau protein plays an important role in microtubule stabilization and axonal transport. The accumulation of NFTs in neurons directly impacts microtubule dysfunction and neuronal degeneration. These studies found that hyper-phosphorylated tau proteins dissociate from the microtubules, significantly decreasing microtubule stability, even causing the neurons to lose their main transport functions and viability. In this study, we seek to understand the molecular mechanism underlying the aggregation of hyperphosphorylated tau proteins. Since hyperphosphorylated tau proteins are highly negatively charged, electrostatic repulsion occurs, hindering their aggregation. This means that they need counterions, positively charged molecules, to compensate for the charge imbalance and promote aggregation. Here, the results showed that tau aggregation is primarily driven by electrostatic interactions with positively charged polyamines, while metal cations including Mg^{2+} and Zn^{2+} play a considerably smaller role. More interestingly, it was confirmed that there was a synergistic effect in tau aggregation with a mix of polyamines and metal cations.

Poster Presentation : **PHYS.P-146**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Studies of photo-reversible fluorescent hydrogel with pdDronpa: Synthesis and characterization

Yeonji Kim, Namdoo Kim[1,*]

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

Dronpa145N is a tetrameric fluorescent protein undergoes reversible photo-switching and photo-dissociation by cyan light (dissociation) and violet light (re-association). pdDronpa is a dimeric derivative of Dronpa145N which is bright and more sensitive to light while forms less aggregates both in vitro and in vivo. We synthesized light-controllable fluorescent hydrogel with polyethyleneglycol (PEG)-maleimide and pdDronpa. This hydrogel showed reversible gel-sol transition under cyan light and violet light. Then, we added restriction enzyme-treated lambda DNA fragments during hydrogel synthesis. After cyan light illumination, DNA fragments were able to escape from the hydrogel, and DNA chelating dye could bind to them resulting in strong red fluorescence.

Poster Presentation : **PHYS.P-147**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

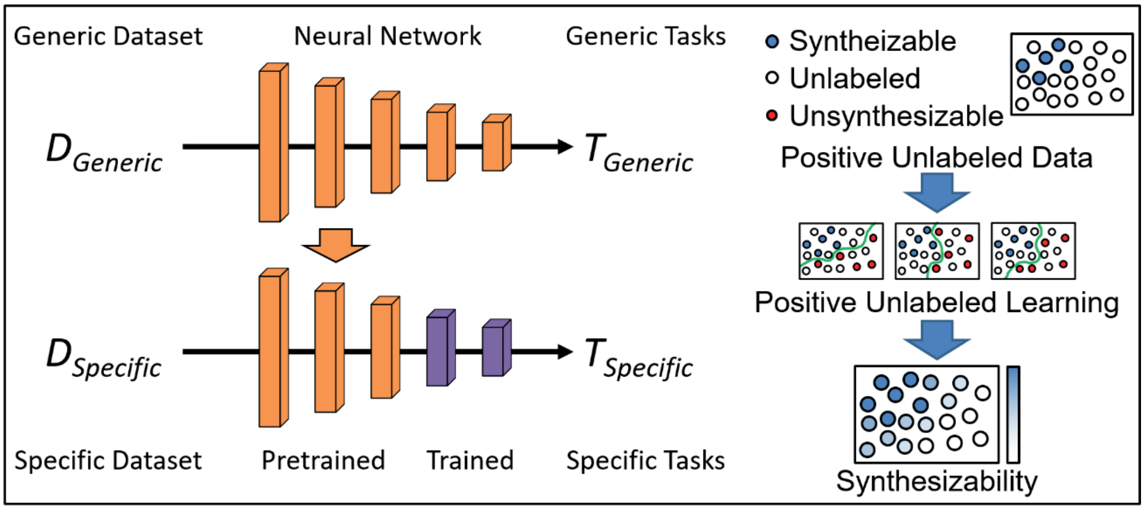
Domain-Transfer Exploration of Perovskite Synthesizability with Positive and Unlabeled Learning

Geun Ho Gu, Juhwan Noh[1], Yousung Jung[1,*]

Department of chemical and biomolecular engineering, Korea Advanced Institute of Science and Technology, Korea

[1]*Department of Chemical and Biomolecular Engineering, Korea Advanced Institute of Science and Technology, Korea*

The perovskite is a promising material type for several applications. However, the number of discovered perovskite remains small. To accelerate the high-throughput discovery of perovskites, we implement transfer positive-and-unlabeled learning, that we developed before,[1] to assess the synthesizability of virtually made perovskite crystals.[2] We train our base model using the crystal data in the Materials Project (~120,000), and perform transfer learning with perovskite data from Materials Project, Aflow, and OQMD (~13,000), resulting in a true positive accuracy of 96%. Out of ~12,000 virtually created perovskites, we find that 962 virtual crystals are predicted to be synthesizable. We searched these crystals in the literature and found that 179 crystals have indeed been synthesized before, substantially increasing the pool size of known crystals. Whereas the previous perovskite stability prediction model focused on the classical ionic perovskite, our model is capable of predicting the synthesizability for anti-perovskites, halides, and covalent perovskite. Also, compared to the heuristic-based Goldschmidt factor, our model selectively chooses synthesizable candidates. Finally, we tabulated synthesizable candidates for the Li-rich ion conductors and photoactive metal halide materials. [1] Jang, J., Gu, G. H., Noh, J., Kim, J., and Jung, Y. J. Am. Chem. Soc. 2020, 142 (44), 18836-18843[2] Gu et al. In preparation.


Generic Dataset
Neural Network
Generic Tasks
$D_{Generic}$
$T_{Generic}$
$D_{Specific}$
$T_{Specific}$
Specific Dataset
Pretrained
Trained
Specific Tasks
● Syntheizable
○ Unlabeled
● Unsynthesizable
Positive Unlabeled Data
Positive Unlabeled Learning
Synthesizability

Poster Presentation : **PHYS.P-148**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Adsorption configurations of tetrahydrothiophene on Ge(100) surface

Jeong Min Ha, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

We investigated the adsorption configurations of tetrahydrothiophene on a Ge(100) surface using high-resolution photoemission spectroscopy (HRPES) and density functional theory (DFT) calculations. On the basis of the HRPES spectra, we confirmed the two adsorption species composed of the major structure through the ring-opening reaction and minor S dative bonded structure. Through DFT calculations, the adsorption geometries and transition states for tetrahydrothiophene on the Ge(100) surface were identified. The adsorption energy of minor S dative bonded configuration for tetrahydrothiophene on the Ge(100) surface was calculated as -21.9 kcal/mol. In addition, the three possible transition states of tetrahydrothiophene adsorbed on the Ge(100) surface through interdimer row, intradimer row, and on-top reaction were confirmed. As a result, we found that the major adsorption structure of tetrahydrothiophene on the Ge(100) surface was formed by ring-opening reaction along the interdimer row mechanism with its adsorption energy of -24.2 kcal/mol and corresponding transition state of 7.0 kcal/mol.

Poster Presentation : **PHYS.P-149**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

On line Time-of-flight Mass Analyzer for Fast Monitoring of Process Gases in Semiconductor/Display Device Production

Eui Young Ji, Hyun Sik Kim[1], Kwang woo Jung[2,*]

물리화학/화학과(chemistry department), Wonkwang University, Korea
[1]*Korea Basic Science Institute, Korea*
[2]*Department of Chemistry, Wonkwang University, Korea*

This work is focused on developing a miniaturized time-of-flight mass analyzer (TOFMA) with an electron-impact ionization source. The goal is to achieve a total system solution for online monitoring of the chemical species in the chemical vapor deposition, etching, cleaning processes used to manufacture semiconductor devices in factory sites. A mass resolution of 219 at m/z 614 has been obtained with a total size of 50 × 40 × 30 cm, the weight of 15 kg, and the power consumption of less than 100W. For the fast chemical reaction monitoring during fabrications, a spectral storage rate was increased to 2,000 spectra/s. The portable mass analyzer was also evaluated by analyzing the plasma etching and cleaning gases in the process reactor. The results indicate that the TOFMA will be useful for a wide range of applications, particularly for in situ environmental and process monitoring.

Poster Presentation : **PHYS.P-150**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Characterization of photo-reversible hydrogel using photo-dissociable dimeric Dronpa

Yeeun Jeong, Namdoo Kim[1,*]

chemistry, Kongju National University, Korea
[1] *Division of Chemistry, Kongju National University, Korea*

pdDronpa is a dimeric version of tetrameric Dronpa145N that is photo-switchable and photo-dissociable green fluorescent protein. It has faster kinetics of photo-switching than Dronpa145N by cyan light. In addition, it shows better dissociation and less aggregation which makes it suitable for photo-reversible hydrogel synthesis. We synthesized the hydrogel using 8-armed PEG and pdDronpa for light control. First, we confirmed that resulting hydrogel undergoes gel-sol transition by cyan light and violet light reversibly. Then, we introduced short DNA fragments into the hydrogel to encapsulate them. After cyan light illumination, released DNA were able to meet DNA chelating dye BOBO-3 which emits strong red fluorescence upon binding with DNA.

Poster Presentation : **PHYS.P-151**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Study of photo-reversible hydrogels using photo-dissociable green fluorescent protein Dronpa

Minjeong Kim, Namdoo Kim[1,*]

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

Hydrogels have high water content, porous structure, relatively soft physical properties and characteristics similar to biological tissues. Therefore, hydrogels have been widely studied and applied in biomaterials for cell culture, drug delivery, biosensors, and tissue engineering. Specifically, photo-responsive hydrogels have advantages that we can tune the mechanical properties of hydrogels in real time with minimal invasion by external stimulations. Here, we made photo-reversible hydrogels using pdDronpa, a photo-reversible green protein, and 8-Armed PEG-maleimide. It showed reversible swelling-shrinking by cyan and violet light, respectively. This hydrogel could be applied to light-controllable drug delivery system.

Poster Presentation : **PHYS.P-152**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

The synthesis, characterization and application of gadolinium oxide nanoparticles for theragnostic purposes

Son-Long Ho, Gang Ho Lee*

Department of Chemistry, Kyungpook National University, Korea

Gadolinium oxide nanoparticles have been employed in numerous reports as MRI contrast agents. However, gadolinium oxides are toxic and therefore need to be surface modified to become water soluble for biomedical application. Herein, we reported the synthesis of gadolinium oxide nanoparticles coated with poly(acrylic acid) with high solubility and low toxicity. These nanoparticles possess higher relaxivities than other commercially available gadolinium compounds. Furthermore, we have conjugated linear RGD to these nanoparticles to increase the tumor targetability and applied these nanoparticles for gadolinium neutron capture therapy.

Poster Presentation : **PHYS.P-153**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Time-Resolved Femtosecond X-ray Absorption Spectroscopy for the Study of Ligand-Field Effects in a Ruthenium(II) Polypyridyl Complex

Yujin Kim, Rory Ma[1], Jessica Harich[2], Miguel Ochmann[2], Nils Huse[2,*], Jae Hyuk Lee[3,*], Tae Kyu Kim[*]

Department of Chemistry, Yonsei University, Korea
[1]*XFEL Science Team, Pohang Accelerator Laboratory, Korea*
[2]*Institute for Nanostructure and Solid-State Physics, University of Hamburg, Germany*
[3]*PAL-XFEL, Pohang Accelerator Laboratory, Korea*

Ruthenium(II) polypyridyl complexes are widely used photosensitizer which provide a platform for functional complexes. In this study, we studied the photo-induced dynamics of $[Ru(m\text{-}bpy)_3]^{2+}$ (m-bpy = 6-methyl-2,2′-bipyridine) with femtosecond X-ray absorption spectroscopy to unveil the time-dependent spin and charge density upon metal-to-ligand charge-transfer (MLCT) excitation. The analysis of spectra at the Ru L_3-edge reveals a very short MLCT lifetime of 0.9 ps and an internal conversion to the lowest triplet metal-centered state (^{3}MC) which relaxes to the ground state with a lifetime of 400 ps. A combination of global analysis and time-dependent density functional theory (TD-DFT) shows that ligand methylation lowers the ligand field strength and thus stabilizes the ^{3}MC state. Our results indicate that small changes in the ligand field leads to the control of photophysical properties which can be uniquely probed with femtosecond X-ray spectroscopy.

Poster Presentation : **PHYS.P-154**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

The dynamics of probe molecules in polymer thin films and interfacial dynamic length scales

Taejin Kwon, Bong June Sung*

Department of Chemistry, Sogang University, Korea

The thermal and mechanical properties of polymer thin films are different from those of bulk polymers due to the presence of the interfacial mobile layer. For example, previous studies showed that the glass transition temperature of polymer thin films decreases with a decrease in the film thickness because the interfacial mobile layer is more dominant in thinner polymer films. Therefore, measuring the thickness of the interfacial mobile layer is crucial to understanding the unique properties of polymer thin films. Many previous studies have used probe molecules to investigate the interfacial mobile layer in polymer thin films. However, recent studies have shown that introduced probe molecules could be unequally distributed in polymer thin films, which affects the measurement of the thickness of the interfacial mobile layer using probe molecules. In this work, we perform the coarsed-grained molecular dynamics simulations for probe molecules in polymer thin films. We employ the bead-spring polymers and model probe molecules as dumbbell dimers. We show that the probe dimers are mainly located at the surface layer in polymer thin films, which means that the probe dimers mainly reflect the dynamics of the surface layer in polymer thin films. Also, we show that the mobility at the surface layer in polymer thin films is much faster than the mobility at other regions in polymer thin films. These results cause that the measurement using probe molecules could overestimate the thickness of the interfacial mobile layer. One must be careful when the thickness of the interfacial mobile layer in polymer thin films is measured using the probe dimers.

Poster Presentation : **PHYS.P-155**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effects of Polarizability of Ions on their Rotational Diffusion in Organic Ionic Plastic Crystals

Seowoo Park, Bong June Sung[1,*]

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

The organic ionic plastic crystals (OIPCs) are composed of molecular ions and have been considered as a strong candidate for the solid electrolytes of all solid-state batteries. The desired solid electrolytes not only need to be resistant to pressure and temperature variations but also should be electrically conductive. Due to the tremendous viscosity of solid electrolytes, however, it is a formidable task to achieve high electrical conductivity. The rotational motions of ions in OIPCs may be activated at a certain temperature range, which facilitates the diffusion of lithium ions even in solid phases and enhances the conductivity. It has been known that the rotational diffusion of ions in OIPCs are spatially heterogeneous: some ions rotate via hopping motions by a certain angle while others do not. Molecular simulations are successful approaches, which allows us to investigate the rotational diffusion at a molecular level. However, the polarizability of ions has been ignored in the simulation models of previous studies, which should affect the diffusion and conductivity of ions. In this work, we investigate how the polarizability of ions affect the rotational diffusion of OIPCs. We perform atomistic molecular dynamics simulations of 1-methyl-3-methylimidazolium hexafluorophosphate ([MMIM][PF_6]) at temperatures from 75 to 500K under isothermal-isobaric conditions (NPT) with and without electronic polarization to investigate polarization effect on the OIPCs. Polarization increases the density of [MMIM][PF_6] only slightly. We find, however, that polarization induces a faster rotational relaxation, which will certainly enhance the diffusion and the conductivity of lithium ions in OIPCs.

Poster Presentation : **PHYS.P-156**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Plasmon-Driven C-B Bond Cleavage in Nanogaps

Ly Thi Minh Huynh, Sangwoon Yoon*

Department of Chemistry, Chung-Ang University, Korea

Boronic acids are the key compound in the Suzuki coupling reactions and in the detection of monosaccharides. The C–B bond cleavage deboronation is an important side reaction that lowers the Suzuki coupling reaction yield and even disables the saccharides detection. Here we report that protodeboronation occurs for 4-mercaptophenylboronic acid (MPBA) within narrow nanogaps between gold nanoparticles (AuNPs) and planar gold substrates. Irradiation of such nanoparticle-on-mirror (NPoM) systems at 785 nm drives the protodeboronation reaction to form benzenethiol (BT). The wavelength-dependence experiments, combined with the dark-field single-particle scattering spectroscopy, reveal that excitation of the bonding dipole plasmon mode of the NPoM leads to the best efficiency. Among the excited plasmon decay pathways, it is generation of hot charge carriers that induce the protodeboronation reaction of MPBA. The possibility of plasmonic thermal reactions is ruled out because external heating of the substrates does not cause the reaction. Comparison of the reaction yield under the ambient, Ar, and oxygen gas conditions reveals that hot charge carriers transfer to MPBA, which subsequently produces BT, but the presence of oxygen promotes the reaction by opening another hot-electron transfer channel. The protodeboronation reaction of MPBA is an important addition to the catalog of plasmon-driven chemical reactions not only because the reaction is relevant to organic and analytical chemistry, but also because it deepens understanding of the hot carrier dynamics at the interface between plasmonic nanoparticles and molecules.

Poster Presentation : **PHYS.P-157**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Charge Delocalized State and Coherent Vibrational Dynamics in PBI H-aggregates

Seongsoo Kang, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Herein, we present an unprecedented experimental demonstration and structure-property relationship on coherent exciton dynamics and its related vibrational signatures of columnar dye stacks with their H-type exciton coupling. Supramolecular dye assemblies have received attention as a medium for the efficient transport of excitons and charge carriers for widespread applications in artificial light-harvesting systems, organic photovoltaics, and organic solar cell. In this context, supramolecular model systems facilitate to unveil appearing functionalities not seen in its constituent molecules. In a sharp contrast with stacks with J-type exciton coupling, however, the detailed observation of exciton dynamics in H-type aggregates has remained challenging because of the small oscillator strength of Frenkel state and the weak fluorescing nature of the energetically lower-lying state. Using femtosecond transient absorption and time-resolved impulsive stimulated Raman scattering measurements, we succeed in observing the excited state dynamics of self-assembled perylene bisimide (PBI) H-aggregates in two points of view: a) the intermolecular interactions between PBI units in H-aggregates induce the formation of new excited-states, excimer and delocalized radical anion states, and b) the intermolecular out-of-plane along the stacking axis and the PBI core C=C stretch Raman modes can be a vital evidence to grasp the coherent exciton dynamics in H-aggregates.

Poster Presentation : **PHYS.P-158**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Incident angle dependence of Ar^{+} ion for sputtering yield of tungsten

Tae Hyun Kwon, Jeong-Woo Nam, Young-Sang Youn[*]

Department of Chemistry, Yeungnam University, Korea

The effect of sputtering incident angle on sputtering yield for tungsten samples fabricated from different particle sizes of $^{+}$ ions. We confirmed that the surface roughness of 0.1 μm for a tungsten pellet with particle size of $^{+}$ ions accelerated at 1.5 and 2.0 keV. With the increase in incident angle of Ar^{+} ions, the sputtering yield for tungsten sample with particle size of $^{+}$ ions.

Poster Presentation : **PHYS.P-159**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

A-site Ion Exchange Mechanism in FAPbI3/CsPbI3 Perovskite Quantum dot thin films with applied voltage

Yeonsu Woo, YeJi Shin[1], Seog Joon Yoon*

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

Perovskite quantum dots (PQDs) had extended the scalability of perovskite materials with high crystallinity in the colloidal state, band gap tunability, and surface ligand driving capabilities across optoelectronics and photovoltaic cells. However, defect control had emerged as a key to the increased PQDs surface area for improved PQDs performance in optoelectronic applications. FAPbI3 (FA, formamidinium) PQDs are stable but have low photoluminescence quantum yield (PLQY), CsPbI3 PQDs are relatively unstable but have high PLQY. So, giving variety to the composition ratio between two materials enhanced stability and high PLQY. In this work, we approached the effect of applied electrical field to the bilayer of FAPbI3 and CsPbI3 PQDs thin film. We utilized in-situ UV-Vis. Absorption and fluorescence spectroscopic tools to monitor composition changes. We demonstrated the effect of applied electrical field to the bilayer of FAPbI3 and CsPbI3 PQDs for their A-site cation exchange process. These findings can help develop a strategy for enhancing the operational performance of PQDs for optoelectronic devices.

Poster Presentation : **PHYS.P-160**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Rational design of Pt/C electrocatalyst using pulsed laser technique in various solvents and their electrochemical performance towards in hydrogen evolution reaction

Yujeong Jeong, Yiseul Yu, Hyeyeon Lee, Theerthagiri Jayaraman, Seung Jun Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Hydrogen is a promising energy source for green energy applications due of its high energy density, negligible pollution and carbon free by-products. In the demand of electrical energy, large-scale hydrolysis for producing high-purity hydrogen is attracting attention. Recently, preparation of novel electrode material for the generation of hydrogen with low overpotential has been motive area of research. It is well known that Platinum (Pt) is a state of the art material for her with lower overpotential and high H_{ads} capability. Electrocatalyst for hydrogen production having extremely low amounts of platinum (Pt) could make cost-effective and state-of-the-art material for water splitting. Herein, we report a one-pot synthesis of carbon-encapsulated Pt nanoparticles (Pt/C) NPs by targeting Pt plate in various solvents such as DI water, methanol, ethanol and 1-propanol using pulsed laser ablation (PLA) technique. The effect of solvents on the size of Pt NPs and carbon layer was systematically examined. The synthesized Pt/C nanocatalysts were characterized using various techniques such as UV-visible, Raman spectroscopy, FE-SEM and HR-TEM analysis. Linear sweep voltammetry (LSV) and Tafel plot were used to evaluate the performance of various Pt/C electrocatalyst for hydrogen evolution. Detailed electrochemical investigation revealed that Pt/C obtained from an ethanol solvent exhibit current density of 10 mA cm^{-1} at 97 mV of overpotential in acidic medium. Therefore, this study revealed a low-cost and single-step synthesis of Pt/C using pulsed laser technique with varieties of solvents could be as a promising electrocatalyst and can act as replacement for commercial Pt/C.

Poster Presentation : **PHYS.P-161**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Introduction of PbSO4-Oleate Capping Layer for Selective Control of Halide ion Migration at CsPbX3 (X = Cl-, Br-, and I-) Quantum Dots.

Yeonsu Woo, Seog Joon Yoon[1,*]

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

Selective control of halide ion exchange in metal halide nanocrystals (NCs) plays an important role in determining the bandgap and composition of nanocrystals. The CsPbX3 (X = Cl-, Br-, and I-) NCs were self-assembled with PbSO4-oleate to form as peapod-like morphology to control halide ion exchange selectively. By utilizing the distinct absorption and bright luminescence characteristics of these NCs, in-situ UV-Vis. absorption and fluorescence spectroscopic tools were utilized to monitor time-dependent band gap and composition changes of the NCs. Unlike non-capped NCs and their rapid anion exchange, we figured out the halide exchange is dependent on morphology of peapod on the NCs. Depending on the morphological change, we tracked the halide ion exchange between two CsPbBr3 and CsPbI3 NCs through the in-situ UV-Vis. absorption/photoluminescence spectroscopies. We were able to regulate the halide exchange reaction rate with the presence of the peapod-like PbSO4-oleate coverage on the NCs. We monitored that the coverage change halide exchange kinetics and activation energy. These results can be attributed to white-LEDs, photo-voltaic cells, and photocatalysts using the divalent composition of the CsPbX3 NCs for alternative structural designs.

Poster Presentation : **PHYS.P-162**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Label-Free SERS Strategy for detecting Amyloid beta-42 on Silver Nanoshells

Eun Hae Heo, Eungyeong Park[1], Hyejin Chang[*]

Division of science education, Kangwon National University, Korea
[1]*Department of Chemistry, Kangwon National University, Korea*

Alzheimer's disease (AD) is the most common on neurodegenerative disorder, and level of amyloid beta 42 (Aβ_{42}) is considered one of the major neuropathologic biomarkers for AD. Herein, a label-free strategy using surface enhanced Raman spectroscopic (SERS) platform is reported for developing an Aβ_{42} sensor. Using the strong affinity of Aβ_{42} and Cu^{2+}, we designed Ag nanoshell-*p*-aminothiophenol (ATP)-Cu^{2+} system. Our sensor showed low selectivity for other proteins, and the sensing effect was confirmed by changing the metal ion and the substituent of aromatic thiol. Details of the results will be discussed in the presentation.

Poster Presentation : **PHYS.P-163**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Role of Electric Field for Formamidinium Lead Halide Hybrid Perovskite Quantum Dots

Kyoungsoo Kim, YeJi Shin[1], ChaeHyun Lee[1], Seog Joon Yoon[1,*], Donghoon Han[*]

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

Organic-inorganic hybrid perovskites have been utilized in optoelectronic applications such as displays, solar cells, and nonlinear optics. Hybrid perovskites contain various components with high polarity and/or charge values, which undergo transformations due to ion exchange, photoinduced phase segregation, or ion migration. These variable characteristics make perovskites “soft materials”. Meanwhile, optoelectronic devices often operate under electrochemical conditions in the presence of an electrical field. To examine the effect of this field on the material/photophysical properties of hybrid perovskites, hybrid $FAPbBr_3$ perovskite quantum dots (PQDs) were synthesized in this study. It was found that electric field played an important role in inducing defect-mediated oxidation/reduction reactions, changing the photophysical properties of hybrid PQDs, and causing their irreversible transformations to various lead halide plumbate complexes. These findings can help develop a strategy for enhancing the operational performance of PQDs for optoelectronic devices.

Poster Presentation : **PHYS.P-164**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Hot Carriers Create a Highly Non-Thermal Vibrational State Distribution of Reactants During the Plasmon-Catalyzed Chemical Reaction

Hyun-Hang Shin, Hankyul Lee, Jaeyoung Jeong, Zee Hwan Kim*

Department of Chemistry, Seoul National University, Korea

Reactants on plasmon-excited nanoparticles undergo unusual reactions impossible with thermal or photochemical activations. It was proposed that such reactivities arise from the vibrationally excited reactants created by the hot carriers of metal. Here we present the direct proof of the as-yet validated central claim, the non-thermal vibrational excitation of the reactant. Under the irraditaion of CW laser (λ_{ex} = 633 nm) of 100 kW/cm^2, the surface-enhanced Ramam spectra (SERS) of reactants undergoing a plasmon-catalyzed reaction reveal that a particular vibrational mode possesses > 10 times larger vibrational quanta expected from the thermalized molecules. We also deduce the excitation rate of ~10^{10} s^{-1}, which is 10^4~10^6 fold larger than those possible with purely optical transitions. About 3 % of reactants remain in excited-states under the steady-state illumination, which can govern the overall reactivity. The mode-specificity of the excitation could be reproduced by the resonant electron-molecule scattering model. Besides the mechanistic validation, the result also provides a new means to realize vibrational control of reactions on metal.

Poster Presentation : **PHYS.P-165**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Cryogenic Ultra-low Frequency Raman Spectroscopy of Size-controlled $CH_3NH_3PbI_3$ Perovskite Quantum Dots

Yeonsu Jeong, Myeongkee Park*

Department of Chemistry, Pukyong National University, Korea

Hybrid organic-inorganic perovskite (HOIP) quantum dots (QDs) shows the simple fabrication, tunability of light absorption wavelengths, and high quantum yield. These advantages make perovskite QDs one of the most promising optoelectronic materials for applications such as light emitting diodes and solar cells. In this poster, we demonstrate (1) the synthesis of $CH_3NH_3PbI_3$ HOIP QDs which have different diameters depending on the ligand concentrations and (2) the size-dependent optical characteristics of QDs using cryogenic ultra-low frequency Raman spectroscopy.*Synthesis and TEM characterizations* $CH_3NH_3PbI_3$ QDs were synthesized by using ligand-assisted re-precipitation method with the different injection volumes of 5.0, 1.0×10, and 2.0×10 μℓ of the ligand. In the TEM studies shown in Fig. 1(a-f), we have shown the ligand quantity dependent QD diameters of 11.8±1.5 nm, 8.3±1.0, and 6.8±0.9, respectively. *Uv-Vis, PL, and Raman characterizations* Figure 1g shows the steady-state absorption and photoluminescence (PL) spectra of QDs of different sizes. The smallest QDs (6.8 nm) shows the PL at 1.77 eV, but the largest one (11.8 nm) shows PL at the lower 1.67 eV which is, interestingly, similar to that of bulk $CH_3NH_3PbI_3$. Figure 1(h) shows our home-built Raman apparatus for the cryogenic experiments. Figure 1(i) shows the Raman spectrum of the 8.3 nm diameter QDs measured at 93 K. We have found three distinctive Raman peaks located at 85.1, 139.5, and 276.4 cm^{-1}. This result is clearly compared to complicated Raman peak assignments shown in other Raman results of single $CH_3NH_3PbI_3$ crystals.(doi.org/10.1038/srep16563).

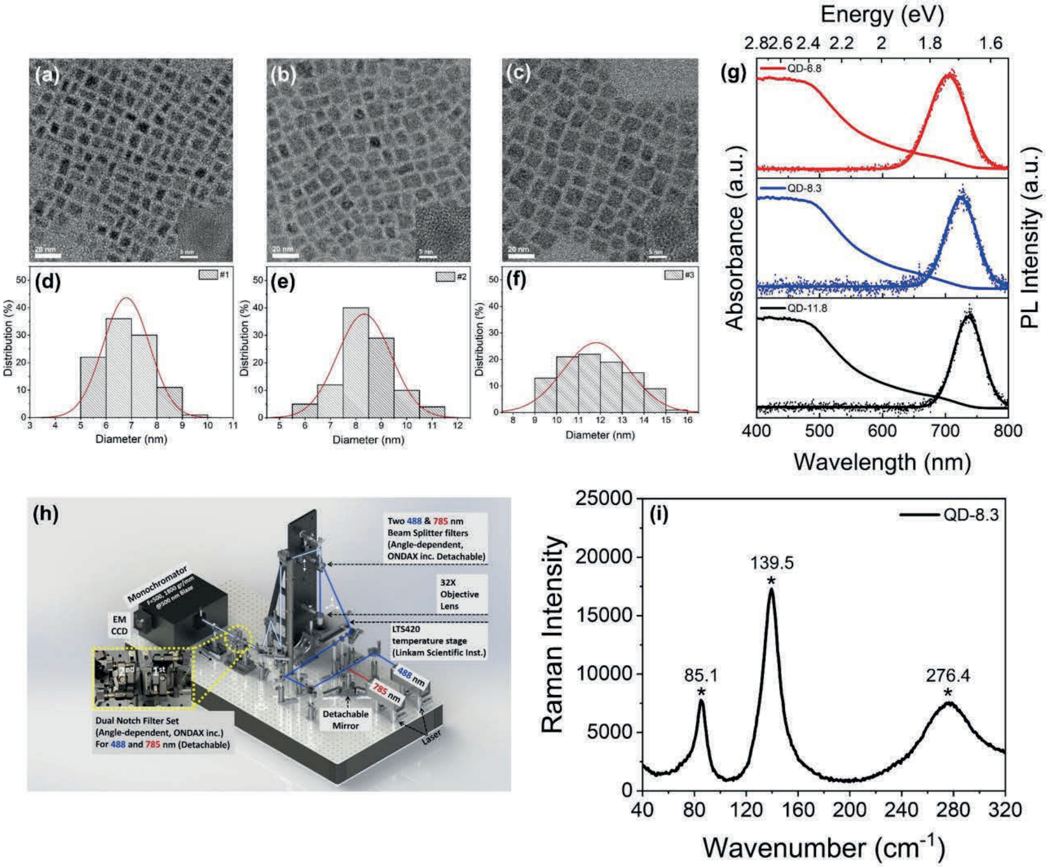


Figure 1. **(a-f)** TEM image and size distributions of $CH_3NH_3PbI_3$ QDs fabricated with oleylamine of 20 $\mu\ell$ (a,d), 10 $\mu\ell$ (b,e) and 5 $\mu\ell$ (c,f). **(g)** UV-Vis absorption and PL spectra of the different size QDs. **(h)** home-built cryogenic Raman spectroscopy. **(i)** Raman spectrum of 8.3 nm-diameter $CH_3NH_3PbI_3$ QD.

Poster Presentation : **PHYS.P-166**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Recovering of the Amplitude and Phase Spectra of a Single Nanoparticle Scattering

Hankyul Lee, Zee Hwan Kim*

Department of Chemistry, Seoul National University, Korea

Interferometric scattering microscopy (iSCAT) is the imaging technique based on interference between a scattered field from a weak scatterer (Escat) and a reflected field from a substrate (Erefl). The iSCAT provides high detection sensitivity and temporal resolution for imaging and tracking of an individual nanoparticle (NP) and a single biomolecule. However, it is hard to be applied to quantitative analysis or spectroscopy because interference signal (Re[Escat*Erefl] of the iSCAT cannot provide separated amplitude and phase information on Escat. Here, we demonstrated a method to recover both the amplitude and phase spectra of an NP-scattered field (Escat) from iSCAT images using Gouy-phase interferometry. The method was validated by showing that the recovered amplitude and phase spectra of a gold nanoparticle fully reproduce well-known spectral features of localized surface plasmon resonances (LSPR).

Poster Presentation : **PHYS.P-167**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Laser-aided synthesis of Zn@ZnO and ZnO for the effective electrochemical sensing of hydroquinone

Juhyeon Park, Ahreum Min, Jiwon Kim, Cheol Joo Moon, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

In this study, Zn@ZnO and ZnO were produced through eco-friendly pulse laser ablation process. The structure, morphology, composition and optical properties of the prepared material were characterized through X-ray diffraction (XRD), Raman spectroscopy, infrared spectroscopy, field emission scanning electron microscopy, high-resolution transmission electron microscopy, UV-vis diffuse reflectance spectrum and photoluminescence analysis. The synthesized Zn@ZnO and ZnO are having high electrical and optical properties. This study illustrate the electrochemical sensing properties of the Zn@ZnO and ZnO towards hydroquinone (1,4-benzenediol). In addition, interference and stability studies were also performed. Competing ions (Na+, K+, Mg2+, Cl-, and NO3-) >100 fold did not interfere with the selective detection of 1,4-benzenediol. Among Zn@ZnO and ZnO based nanocomposites can be effective sensors for the selective and sensitive detection of toxic organic compounds.

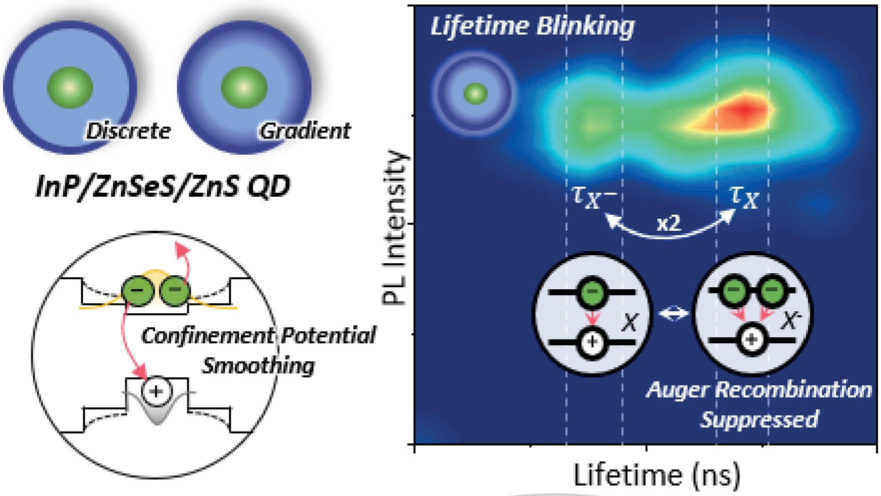
Poster Presentation : **PHYS.P-168**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effect of shell composition and interface engineering on Auger recombination in InP/ZnSeS/ZnS Quantum Dots

Yu Jin Lee, Taehee Kim, Jumi Park[1], Dongho Kim[*]

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

Environment-friendly InP quantum dots (QDs) have attracted immense interest as a promising candidate for self-emitting quantum dot light-emitting diode (QLED) display. In this study, the effects of shell structure and composition engineering on the photoluminescence (PL) properties of InP/ZnSeS/ZnS QDs are investigated. Substantial suppression of the nonradiative Auger recombination, which is one of the major drawback factors in QLED efficiency, is achieved. Ensemble and single–dot analysis reveal that gradient shell QDs with optimal composition smoothens the confinement potential and observes the 'lifetime blinking' phenomenon as charged QDs are luminescent just as neutral QDs. Single QD measurements show that adding gradience in shell structure decreases spectral diffusion and single–dot PL peak width due to the decrease in lattice mismatch between the shells and increases in energy barrier for charge trapping. However, an increase in ZnS composition in the gradient shell (ZnS% > 0.5) reduces the QD performance because of the lattice difference between the core and the shell.


Discrete
Gradient
InP/ZnSeS/ZnS QD
Confinement Potential Smoothing
Lifetime Blinking
PL Intensity
τ_{X^-}
x2
τ_X
X
X⁻
Auger Recombination Suppressed
Lifetime (ns)

Poster Presentation : **PHYS.P-169**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Development and verification of conformer-specific vibrational spectroscopy

Sung Man Park, Chan Ho Kwon[1,*]

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

Conformers have similar vibrational structures both in neutral (S_0) and cationic (D_0) states, owing to the comparable force fields between their nuclei. Nevertheless, there is a continuous development of vibrational spectroscopic techniques to rigorously identify individual conformers in the designated molecule but only in the S_0 state. We developed the inventive conformer-specific vibrational spectroscopic technique capable of measuring the identifiable vibrational spectra of individual conformers in both S_0 and D_0 states using the IR resonant vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy. In addition, we verified the proposed technique by measuring the isomer-specific vibrational spectra of the binary mixture of acetone and oxetane isomers in both states, which can be properly represented by the IR resonant VUV photoionization and the one-photon VUV-MATI spectra of the mixture, under the supersonic expansion condition. The measured IR dip VUV-MATI and IR depletion VUV-MATI spectra of the binary mixture correspond to the isomer-specific vibrational spectra in both states, respectively. Moreover, the estimated partial pressures of the individual isomers in the binary mixture with different mole fractions based on relative peak intensities in the measured spectra give insights on the solute-solvent interaction, and ensures that the inventive spectroscopic technique is applicable in conformational chemistry.

Poster Presentation : **PHYS.P-170**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Individual conformers in C_4H_6O isomers by conformer-specific vibrational spectroscopy

Sung Man Park, Hyojung Kim[1], Chan Ho Kwon[1,*]

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

Conformer-specific vibrational spectra of C_4H_6O isomers (crotonaldehyde (CA) and methyl vinyl ketone (MVK)) in neutral and cationic states were measured using the invented IR resonant vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy. Notably, the measured IR dip and hole-burn VUV-MATI spectra for each isomer represent the identifiable vibrational spectra of individual conformers in both states. Moreover, we estimated the relative populations of individual conformers in CA and MVK isomers using the IR dip intensity, the corresponding Franck–Condon factor, and the IR absorption cross section. Our analysis revealed that the compositional ratio of s-*trans* to s-*cis* conformers in the CA isomer remained at 95.8:4.2 even under supersonic expansion, whereas that in the MVK isomer was determined as 90.6:9.4, which are consistent with previous research. This findings reveal that the conformational stability of each isomer depends on the position of the methyl group relative to the carbonyl group.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **PHYS.P-171**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced electrochemical performance of Nanoalloys Using Pulsed Laser Irradiation

Yiseul Yu, Theerthagiri Jayaraman, Seung Jun Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Recently, more attention has been given for the electrocatlyst to replace platinum based materials. Which is state of the art material for HER generation. In this study, we successfully synthesized AuPt alloy using metal salts in the absence of surfactant and reducing agents through pulsed laser irradiation (PLI) method under the influence of ultra-sonication. The PLI method for preparation of metal NPs and alloys are not been explored well. The range of stoichiometric ratio of metals (Au and Pt) in the alloy was studied towards hydrogen evolution reaction (HER). The formation of alloy provides better run stability and electrochemical performance in HER than single metal NPs. The high-efficiency hydrogen evolution reaction suggests that alloy NPs formed well using robust PLI technique, which can be used as excellent catalysts in terms of electrochemical studies.

Poster Presentation : **PHYS.P-172**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Modulations of a Metal–Ligand Geometry and Photochemical Reactions by Hückel–Möbius Aromatic Switching

Jinseok Kim, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

In organometallic complexes containing pi-conjugated macrocyclic chelate ligands, metal–ligand geometry significantly affects metal-ligand electronic interactions, hence tuning properties of the complexes, since the p- and d-□ orbital hybridizations are pivotal to the metal–ligand interactions. In this regard, we investigated the metal–ligand interactions in hexaphyrin mono-Pd(II) complexes Pd[28]M and Pd[26]H, which exhibits a redox-induced switching of Hückel–Möbius aromaticity and molecular conformation, and their effect on the electronic structure and photochemical reactions. In Möbius aromatic Pd[28]M, a heavily twisted structure leads to weak metal–ligand interactions and leaves the pi electronic structure of the hexaphyrin ligand almost intact, which undergoes efficient intersystem crossing (ISC) assisted by the heavy-atom effect of Pd metal. In Hückel aromatic Pd[26]H, its planar ligand structure allows an effective d-p hybridization, making ligand-to-metal charge-transfer (LMCT) a dark state in the decay of the excited state. These contrasting metal-ligand electronic interactions have been indicated by photoexcited-state dynamics, time-dependent DFT calculations, and transient infrared (TRIR) spectra. This work indicates that the modulation of Hückel–Möbius geometries can effectively manipulate molecular properties of metal complexes, and further enabling the fine-tuning of metal–ligand interactions and the novel design of functional organometallic materials.

Poster Presentation : **PHYS.P-173**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Overtone vibrational excitation of adsorbates driven by plasmonic hot electrons

Hyun-Hang Shin, Jaeyoung Jeong, Zee Hwan Kim*

Department of Chemistry, Seoul National University, Korea

It has been proposed that hot electrons induced by the relaxation of localized surface plasmon(LSP) may transfer vibrational energy to reactans, subsequently induce the activation of the chemical reaction. However, plasmon-induced vibrational excitation and its relation with plasmon-catalyzed chemical reaction have not been directly validated. Employing the surface-enhanced Raman scattering (SERS), we have verified the substantial vibrational excitation of the reactant, 4-nitrobenzenethiol(4-NBT) placed between thin gold film(10 nm) and silver nanosphere(80 nm). In particular, we found that for νNO_2 mode(symmetric N-O stretch of nitro group) of the reacting 4-NBT, the anti-Stokes peak shows broad and asymmetric lineshape that is distinctly different from its Stokes peak and anti-Stokes peaks of other modes. This feature reflects the generation of overtone excited vibrational states of reactants. The lineshape analysis, which takes into account the anharmonicity of the mode, allows us to deduce the vibrational state distribution of the νNO_2 mode. The distribution reveals non-neligible (8 %) population of $v > 5$. Such overtone-excited reactants have internal energy as large as the known activation energy for conversion of 4-NBT to 4-aminobenzenethiol, supporting the claims that vibrationally hot reactants are responsible for the observed plasmon-catalyed reaction.

Poster Presentation : **PHYS.P-174**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Mathetmatical model of microbial consortia with genetic circuit for improved biochemical production

Jaehyuk Won, Ji-Hyun Kim*, Jaeyoung Sung*

Department of Chemistry, Chung-Ang University, Korea

Microbial consortia have been considered potential platforms for bioprocessing applications. However, the complexity in process control owing to the use of multiple strains necessitates the use of an efficient population control strategy. Herein, we report circuit-guided synthetic acclimation as a novel strategy to improve biochemical production by a microbial consortium. We designed a consortium comprising alginate-utilizing Vibrio sp. dhg and 3-hydroxypropionic acid (3-HP)-producing Escherichia coli strains for the direct conversion of alginate to 3-HP. We introduced a genetic circuit, named “Population guider”, in the E. coli strain, which degrades ampicillin only when 3-HP is produced. We modeled the consortium mathematically to prove the circuit-guided population control improves biochemical production. It is shown that the present theory can predict optimized strain population ratio for efficient metabolite production

Poster Presentation : **PHYS.P-175**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Investigation of the effect of dsDNA bending on Z-DNA by single-molecule FRET

Jaehun Yi, Nam Ki Lee[1,*]

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

Z-DNA, a non-canonical helix form of double stranded DNA (dsDNA), plays an essential role in biological processes such as transcription regulation. In previous research, Z-DNA could be formed under mechanical stress such as negative supercoiling or tension. However, the effect of dsDNA bending, the most common deformation of DNA in vivo, on Z-DNA formation is still elusive. In order to investigate, we measured single-molecule fluorescence resonance energy transfer via alternating-laser excitation confocal microscopy. We also regulated the bending force on dsDNA without any external forces by a D-shaped DNA nanostructure. Herein, we show that dsDNA bending involves in the formation of Z-DNA, as revealed by varying the salt concentration at which Z-DNA is formed depending on the bending force. Thus, our result provides a new insight for the effect of dsDNA bending on transcription regulation through Z-DNA formation.

Poster Presentation : **PHYS.P-176**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Spectroscopic Characterization of Selenium Quantum Dots (SeQDs) at Ultralow Temperature

Jiwon Kim, Ahreum Min, Cheol Joo Moon, Juhyeon Park, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

In this study, we synthesized PbSe, CdSe, and Ag_2Se using pulsed laser irradiation in liquid (PLIL). In particular, Ag_2Se does not contain heavy metals and has excellent thermal conductivity, so it has recently been spotlighted as a next-generation semiconductor material. Using PLIL, an eco-friendly synthesis method, we synthesized three selenium quantum dots (SeQDs) and measured the structural, chemical, and photoelectric properties of synthesized SeQDs. We checked the synthesized SeQDs for shape through SEM, and the particles were analyzed using UV and FT-IR spectroscopy. Furthermore, we confirmed the microelectronic structure and characteristics of SeQDs by measuring the PL spectrum in the NIR region at ultralow temperature and analyzed the spectroscopic characteristics at ultralow temperature by comparing them with the PL at room temperature.

Poster Presentation : **PHYS.P-177**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced Photoelectrochemical Water Oxidation of $BiVO_4$ Photoanode with Co-incorporated Hydroxyapatite Nanoarchitecture as Efficient Oxygen Evolution Cocatalyst

Inae Song, Tae Kyu Kim[1,*]

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

Photoelectrochemical (PEC) water splitting using semiconductor offers a promising strategy to produce the renewable hydrogen energy. Oxygen evolution reaction (OER) on photoanode is a critical half-reaction for overall water splitting because it is the kinetically sluggish process as a four-electron reaction which is hard to take place. Various semiconductors have been applied to the study of PEC water splitting, including Fe_2O_3, TiO_2, $BiVO_4$ and WO_3 etc. Among those semiconductors, Bismuth vanadate ($BiVO_4$) has widely emerged as a promising photoanode because of good stability against photo-corrosion, a narrow band gap of 2.2-2.4 eV which is a proper energy for water splitting. However, some disadvantages such as slow charge mobility and fast recombination restrict low efficiency.Herein, we fabricated an oxygen evolution cocatalysts such as NiFe-layered double hydroxide (NiFe-LDH) and Co-incorporated hydroxyapatite (Co-HAP) nanoarchitecture on $BiVO_4$ to enhance the PEC. The resulting $BiVO_4$/NiFe-LDH/Co-HAP photoanode showed 3.99 mA/cm^2 of photocurrent density at 1.23 V *vs.* RHE under AM 1.5 G illumination in potassium phosphate electrolyte. This was 3.7 times higher than bare $BiVO_4$ photocurrent density which was 1.07 mA/cm^2. Also, the onset potential showed cathodic shift. The improved PEC performance is resulted from the accelerated charge separation/transfer and the inhibited surface charge recombination due to the synergistic effect of NiFe-LDH and Co-HAP.

Poster Presentation : **PHYS.P-178**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Chiral and Isomeric Discrimination of Chiral Molecular Ions by Cold Ion Circular Dichroism Spectroscopy

HanJun Eun, Nam Joon Kim*

Department of Chemistry, Chungbuk Natioanl University, Korea

Circular dichroism (CD) spectra contain information about absolute configurations and conformations of chiral compounds. However, extracting this information from CD spectra in solution is challenging because the spectra exhibit only the averaged CD values of all different conformers. CD spectroscopy of jet-cooled molecules can provide conformation-specific CD spectra, but its application to large biomolecules has been limited due to the difficulty of their production in the gas phase. Here, we obtained the first CD spectra of chiral molecular ions produced by electrospray ionization (ESI) using cold ion CD spectroscopy. Protonated L- or D-phenylalanine ions produced by ESI were stored in a cold quadrupole ion trap and irradiated by multiple laser pulses with left or right circular polarization. The CD spectra exhibited well-resolved CD bands of two conformers, whose signs are opposite to each other. We also have obtained ultraviolet photodissociation (UVPD) circular dichroism (CD) spectra of protonated L-phenylalanyl-L-alanine (L-H+PheAla) near the origin band of the S0-S1 transition using cryogenic ion spectroscopy. These results demonstrate that the CD values of L-H+PheAla near the origin band reflect the different conformations of the Phe side chain. These results will broaden the scope of conformation-resolved CD spectroscopy to large molecular ions without size limitations.

Poster Presentation : **PHYS.P-179**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Analysis of bi-exciton annihilation in emitting layers in OLEDs

Hyoseong Lee, Chang Woo Koh[1], Sungnam Park[2,*]

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

In the OLED devices, bi-exciton annihilation processes, such as singlet-singlet annihilation (SSA), singlet-triplet annihilation (STA), and triplet-triplet annihilation (TTA), need to be avoided or substantially minimized for high performance. Especially, bi-exciton annihilation processes become important at high current densities leading to significant efficient roll-off. In this work, a method for analyzing the bi-exciton annihilation processes occurring in the emitting layers of OLEDs is developed. The PL intensities are measured with host-dopant films as a function of the power of laser excitation. The log-log plots of the PL intensity vs the power of laser allow us to quantify the bi-exciton annihilation. By analyzing the log-log plots of the PL intensity vs the power of laser with the analytic model we developed, the rate constants for SSA, STA, and TTA were readily determined. Our analytic method combined with the power-dependent PL experiments can be effectively used to understand the bi-exciton annihilation processes in the OLED devices.

Poster Presentation : **PHYS.P-180**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Numerical simulation of the external quantum efficiency of OLEDs

<u>Hyoseong Lee</u>, Chang Woo Koh[1], Sungnam Park[2,*]

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

The external quantum efficiency (EQE) of organic light-emitting diodes (OLEDs) is determined by internal quantum efficiency (IQE) and out-coupling efficiency. At the molecular level, the EQE is influenced by the photoluminescence quantum yield (PLQY) and emitter orientation. Therefore, the EQE can be theoretically estimated using the PLQY and orientation of emitters in the emitting layer (EML) of OLEDs. In this work, we have demonstrated that the EQE can be readily simulated for a give structure of OLED device as a function of PLQY and orientation factor of emitters. The PLQY of emitters can be readily measured using the integrating sphere and the orientation factor of emitters can be measured by angle-dependent PL experiments. The simulation results can be used to estimate the maximum EQE for a given device configuration and to optimize the performance of the given OLED device by controlling the orientation of emitters in the EML and improving the balance in the hole and electron mobility in the given OLED device.

Poster Presentation : **PHYS.P-181**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Forward and backward intermolecular charge transfer description using density functional theory

Junseok Kim, Hyungjun Kim[1,*]

Department of Chemisty, Incheon National University, Korea
[1]*Department of Chemistry, Incheon National University, Korea*

The charge transfer (CT) is one of the most important concepts in various chemistry fields such as solar cells, organic synthesis and photocatalysts. Quantum chemistry simulations can provide important chemical insights into charge transfer states. In description of CT state, the lowest-lying CT states, which require the smallest amount of excitation energy to access them, are the main interests of theoretical communities.In most cases of intermolecular charge transfer, the lowest-lying CT states are characterized by the electron transfer from donor to acceptor, which is denoted as forward CT in this study. The recent study showed that the definition of donor and acceptor might be undetermined and depends on the relative orientation especially for the weak donor-acceptor system.[1] Under the certain condition, the electron transfer from acceptor to donor is found as the lowest-lying CT state, which is denoted as backward CT.In this study, we benchmarked the performance of TDDFT with various classes of functionals, global hybrid and range-separated hybrid generalized gradient approximation for the description of forward and backward intermolecular CT. The contribution of Hartree-Fock exchange in DFT functionals, the impact of basis sets enlargement, and the performance of constrained DFT (CDFT) method are mainly discussed. This study suggested a viable function to adequately describe forward and backward CT of intermolecular charge transfer systems within the DFT framework.References[1] C. park, V. Atalla, S. Smith, and M. Yoon, Understanding the Charge Transfer at the Interface of Electron Donors and Acceptors: TTF–TCNQ as an Example. ACS Appl. Mater. Interfaces 2017, 9, 32, 27266–27272

Poster Presentation : **PHYS.P-182**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

One-pot laser assisted Synthesis of M-BTC (M: Cu, Co, Ni) MOF as highly active and structurally robust electrocatalyst for overall water splitting in alkaline condition.

Shreyanka Shankar Naik, Theerthagiri Jayaraman[1], Seung Jun Lee[1], Myong Yong Choi[1,*]

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

The electrocatalytic driven water splitting process is highly necessary alternative for the generation of carbon free fuels. Developing a highly-active and low cost bi-functional electrocatalyst to influence in hydrogen evolution reactions (HER) and oxygen evolution reactions (OER) has important role in water-splitting. Thus, we have successfully synthesized complex nanostructure having various architecture of Cu-BTC, Co-BTC and Ni-BTC MOF materials by new method of pulsed laser ablation (PLA) in mono-solvent DMF medium. As prepared MOF materials were characterized using XRD, XPS Raman, FT-IR, TGA, FE-SEM and HR-TEM analysis. Further, MOF material were utilized for electrochemical reactions, which showed better activities in HER and OER applications in alkaline medium. Among the synthesized MOF materials, the Co-BTC catalyst showed a very low overpotential of 437 mV towards HER at a constant current density of 10 mA cm-2 in 1M KOH. The derived Tafel slope and Rct values are 115.1 mV dec-1 and 2.77 Ω cm-2. Similarly, OER studies reveals that Co-BTC MOF showed robust activity with low overpotential of 370 mV for corresponding current density of 10 mA cm-2. Finally, the best performing modified material of Co-BTC/CC MOF electrode required 2.03V cell potential to deliver 10 mA cm-2 in a di-electrode (Co-BTC/CC II Co-BTC/CC) electrolysis system with long run stability with negliblibe current loss. Thus, we believe that our study reveal a new possibilities for the innovation in HER and OER bifunctional electrocatalyst using monometallic MOF materials.

Poster Presentation : **PHYS.P-183**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Single molecule microscopy with high localization precision in a temperature-controlled vacuum setup for studying translational diffusion of polymer

Soohyun Lee, Keewook Paeng[*]

Department of Chemistry, Sungkyunkwan University, Korea

Single molecule microscopy can be used to study translational diffusion of polymer, based on observations of the trajectories of individual fluorescence molecules. However, low collection efficiency of microscopy setup makes it difficult to determine accurate position of single particle. Therefore, we design new temperature-controlled vacuum setup with high NA objective lens to secure high localization precision by obtaining high collection efficiency. New microscope setup with high NA objective inside vacuum chamber provides 2.5 times higher fluorescence collection efficiency, resulting in about 3 times higher localization precision. Also, we study how localization precision changes according to magnification, EM gain, and exposure time, which can change pixel size, total number of photons, and background noise. This new microscope setup with high localization precision make it possible to measure slower translational diffusion up to lower temperature, which could not be measured before.

Poster Presentation : **PHYS.P-184**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Janus spherical Pt@MXene composite by using pulsed laser irradiation in Aqueous Media

Hyeyeon Lee, Chae Eun Park, Gyoung Hwa Jeong, Seung Jun Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

A titanium carbide nanosheet having a two-dimensional flat structure similar to graphene can be made by selectively melting an aluminum element in a "Ti3AlC2" three-dimensional crystalline material called MAX. This material is called MXene, and it has potential applications as electromagnetic wave blocking materials, energy storage materials, composites for strengthening materials, and catalysts. In order to overcome the toxicity and enormous cost of conventional methods, it is essential to develop an eco-friendly and reliable nanomaterial production process. This produced MXene Pt composites by second harmonic pulsed laser irradiation and sonication. Various analytical techniques from HR-TEM, SEM, XRD, Raman, XPS studies were used to confirm the formation of MXene Pt complexes. And its applicability as an electrochemical and organic reaction catalyst is being studied.

Poster Presentation : **PHYS.P-185**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Shape- and Size-Controlled Palladium Nanocrystals and Their Electrocatalytic Properties in the Oxidation of Ethanol

Hyeon Jeong Kim, Young Wook Lee[1,*]

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

Pd nanoparticles (PdNPs) were synthesized in an aqueous environment via the reduction of K_2PdCl_4 by a surfactant under a high temperature. Highly monodisperse spherical PdNPs and multi-pod PdNPs with a controlled size ranging from 18 to 50 nm were prepared in high yields by varying the concentration of cetyltrimethylammonium chloride. The structural and optical properties of the synthesized Pd NPs were characterized by transmission electron microscopy, X-ray diffraction and UV–vis spectroscopy. The spherical and multi-pod PdNPs exhibited catalytic properties that were unique to their size and shape and presented efficient electrocatalytic activities toward the ethanol oxidation reaction.

Poster Presentation : **PHYS.P-186**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Active Site Rich Multifunctional Ni–CuO Nanocomposites by Pulsed Laser Ablation for Boosting Methanol Electro-Oxidation and Overall Water Splitting

Talshyn Begildayeva, Seung Jun Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Multifunctional electrocatalysts are vital for energy conversion and storage applications. Here a novel laser-based synthesis method for the preparation of multifunctional Ni–CuO nanocomposites, which can be utilized in methanol oxidation reactions (MOR), oxygen and hydrogen evolution reactions (OER and HER), is discussed. The growth mechanism of CuO in presence of Ni NPs, as well as the corresponding effects on the electrocatalytic activity, are studied. The prepared electrocatalyst exhibits trifunctional catalytic activity. The controlled change of the CuO nanorods into nanospheres with more electrochemically accessible Cu sites in presence of Ni NPs results in excellent MOR activity with a high current density of 10.21 $mAcm^{-2}$ at the vertex potential. Moreover, the electrocatalyst displays high turnover capability and stability in OER and HER. It is demonstrated that Ni–CuO can potentially be used as a water splitting electrocatalyst in alkaline conditions. This work shows that the method of pulsed laser ablation can be employed for the development of efficient and stable multifunctional electrocatalysts.

Poster Presentation : **PHYS.P-187**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Recent Study on the Topology of Vitamin K Epoxide Reductase

Sangwook Wu*, **Suhyun Park**

Department of Physics, Pukyong National University, Korea

Vitamin K epoxide reductase (VKOR), key enzyme for blood coagulation, is the target of themost widely prescribed oral anticoagulant warfarin. Recently, the warfarin binding to the humanVKOR (TY139A) is revealed by using molecular dynamics simulation for three transmembranemodel (3TM). QM/MM calculation veri

es a coupled state between the benzene ring of the warfarinmoiety and the benzene ring of Y139 at electronic level. Recently, VKOR (4TM) structure boundto warfarin is x-ray crystalized. We discuss about possible binding modes of warfarin to the humanVKORs with different topology.

Poster Presentation : **PHYS.P-188**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Two-photon Absorption Cross-section Study of *pyrazino[2,3-g]quinoxaline* derivatives by using Z-scan technique

Nurwarrohman Andre Sasongko, Jiwon Choi, Myeongkee Park[*], Songyi Lee[*]

Department of Chemistry, Pukyong National University, Korea

Two-photon absorption (TPA) is the optical process where an electron absorbs two-photon to move from the ground state through a virtual state or intermediate to the excited state. Currently, studying organic molecules to have large TPA cross-sections is very significant for the potential applications in cell imaging, sensing, and optical storage devices. Here, we have study *pyrazino[2,3-g]quinoxaline*(PQ) which is a general fluorescent material having donor-π-acceptor system, largely used in TPA microscopy due to their large TPA cross-sections at lower than 800 nm. (Figure 1)In this work, we describe the (1) experimental z-scan technique of a small organic molecules-based *pyrazino[2,3-g]quinoxaline*. We also demonstrate the (2) relations between molecular structures and TPA cross-sections value by fitting z-scan data using equation 1, where β is two-photon absorption coefficient, I_0 is the intensity at the focus, L is the sample thickness, and z_0 is diffraction length. The highest TPA cross-section (1870 GM@778 nm) is found in *2,3-diethylpyrazino[2,3-b]phenazine*(DS2). This result depicts that there is no significant effect on the acceptor group. It is even larger than that of Rhodamine B (~150 GM@800 nm). Moreover, this investigation describes that the phi conjugation does not affect the TPA cross-sections, although the maximum wavelength increase. These high TPA cross-sections in the DS series and detailed structure correlations show that organic molecule-based *pyrazino[2,3-b] phenazine* without heavy atoms can be very promising for TPA imaging.

$$T(z) = 1 - \frac{\beta I_0 L}{2^{3/2}\left(1+\left(z^2/z_0^2\right)\right)} \quad (1)$$

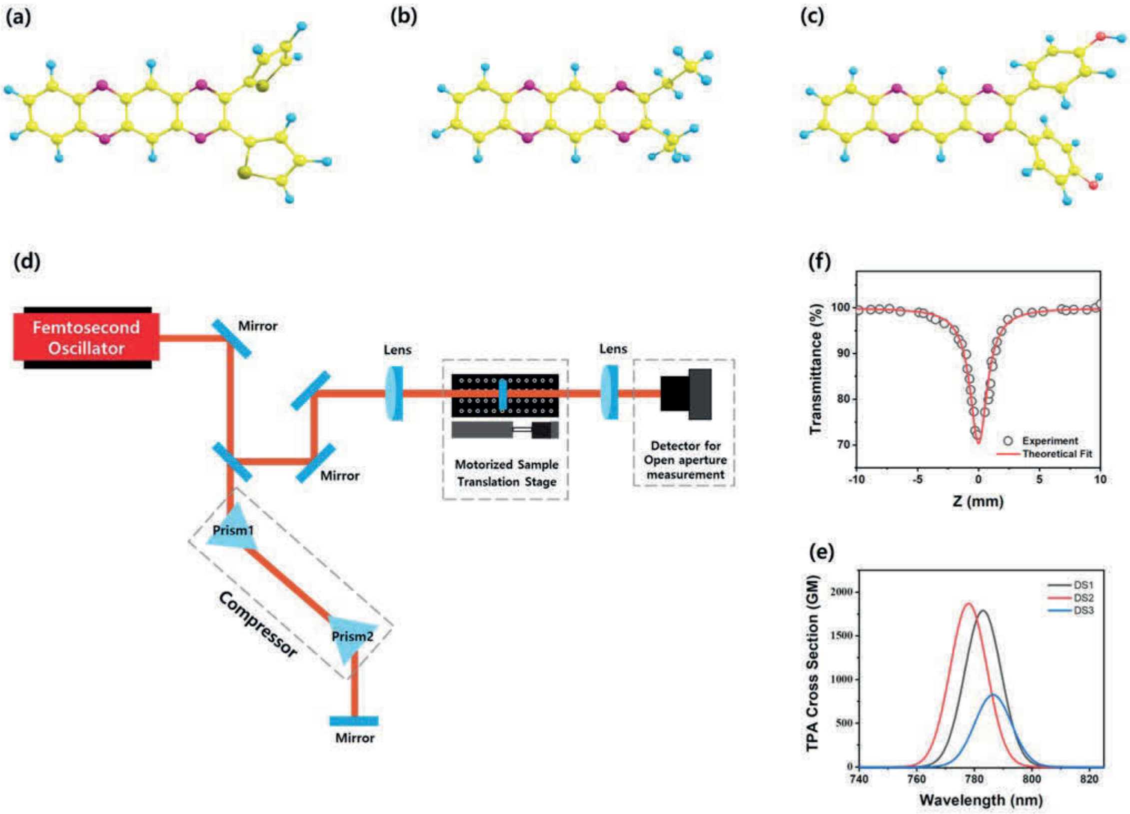


Figure 1. Molecular structure of (a) DS1, (b) DS2, (c) DS3. (d) Schematic z-scan setup for third-order nonlinearity characterization. (e) Open aperture z-scan trace of DS3 in the spectral range of 720–820 nm. (f) Two-photon absorption spectra of DS1 (red-line), DS2 (black-line), DS3 (blue-line) in the spectral range of 720–820 nm

Poster Presentation : **PHYS.P-189**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Photoconversion of Cyanine5 to Cyanine3 and its application high-density single-particle tracking

HyeongJeon An, Chulbom Lee[1,*], Nam Ki Lee[1,*]

Department of Physics, Pohang University of Science and Technology, Korea
[1]*Division of Chemistry, Seoul National University, Korea*

Cyanine (Cy) dyes are among the most useful organic fluorophores that have been used in a wide range of applications in single-molecule and super-resolution imaging as well as in other biophysical studies. However, recent studies that blueshifted derivatives of Cy dyes are formed via photoconversion have raised concerns as to the potential artifacts in multicolor imaging. Here, we report the mechanism for the photoconversion of Cy5 to Cy3 that occurs upon photoexcitation during fluorescent imaging. Our studies show that the formal C2H2 excision from Cy5 occurs mainly through an intermolecular pathway involving a combination of bond cleavage and reconstitution, while unambiguously confirming the identity of the fluorescent photoproduct of Cy5 to be Cy3 using various spectroscopic tools. We also show that the deletion of a two methine unit from the polymethine chain, which results in the formation of blueshifted products, commonly occurs in other cyanine dyes, such as Alexa Fluor 647 (AF647) and Cyanine5.5. We demonstrate that the potentially deleterious photoconversion, however, can be exploited to develop a new photoactivation method for high-density single-particle tracking in a living cell without using UV illumination and cell-toxic additives.

Poster Presentation : **PHYS.P-190**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Gel-sol transition and material transfer using optical switch hydrogels.

Sanghyeuk Son, Namdoo Kim*

Division of Chemistry, Kongju National University, Korea

Sanghyeuk SonDepartment of chemistry, Kongju National Univercity, Gongju 32588, Republic of KoreaCurrently, the methods of using hydrogel to transfer substances are diversifying. The physical properties of hydrogel can be controlled by adding substances that react to a given stimulus from the outside. Among them, hydrogels were produced using pdDronepa and PEG, which respond to 405 nm and 505 nm light. First, we studied gel-sol metastasis because the purpose is to transfer substances. Then DNA and BOBO were used to verify that the substance was transmitted accurately without changing. Fluorescent microscopes were used during material transfer experiments.

Poster Presentation : **PHYS.P-191**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

On Internal Conversion between Bright (11B+u)and Dark (21A−g) States in s-trans-Butadiene and s-trans-Hexatriene

Woojin Park, Cheol Ho Choi*

Department of Chemistry, Kyungpook National University, Korea

Internal conversion (IC) between the two lowest singlet excited states, 11B+u and 21A−g, of s-trans-butadiene and s-trans-hexatriene is investigated using a series of single- and multi-reference wave function and density functional theory (DFT) methodologies. Three independent types of the equation-of-motion coupled-cluster (EOMCC) theory capable of providing an accurate and balanced description of one- as well as two-electron transitions, abbreviated as δ-CR-EOMCC(2,3), DIP-EOMCC(4p2h), and DEA-EOMCC(4p2h), consistently predict that the 11B+u/21A−g crossing in both molecules occurs along the bond length alternation coordinate. However, the analogous 11B+u and 21A−g potentials obtained with some multi-reference approaches, such as CASSCF, MRCIS(D), MRCISD+Q, and the linear-response formulation of time-dependent DFT, do not cross. Hence, caution needs to be exercised when studying the low-lying singlet excited states of polyenes with conventional multi-configurational methods and TD-DFT. Among the simplest and least expensive computational methodologies, the DFT approaches that incorporate the contributions of doubly excited configurations, abbreviated as MRSF-TDDFT and SSR(4,4), accurately reproduce our best EOMCC results.

Poster Presentation : **PHYS.P-192**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids

Saima Sadiq, Cheol Ho Choi[1,*]

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

Due to their multiconfigurational nature featuring strong electron correlation, accurate description of diradicals and diradicaloids is a challenge for quantum chemical methods. The recently developed mixed-reference spin-flip (MRSF)-TDDFT method is capable of describing the multiconfigurational electronic states of these systems while avoiding the spin-contamination pitfalls of SF-TDDFT. Here, we apply MRSF-TDDFT to study the adiabatic singlet–triplet (ST) gaps in a series of well-known diradicals and diradicaloids. On average, MRSF displays a very high prediction accuracy of the adiabatic ST gaps with the mean absolute error (MAE) amounting to 0.14 eV. In addition, MRSF is capable of accurately describing the effect of the Jahn–Teller distortion occurring in the trimethylenemethane diradical, the violation of the Hund rule in a series of the didehydrotoluene diradicals, and the potential energy surfaces of the didehydrobenzene (benzyne) diradicals. A convenient criterion for distinguishing diradicals and diradicaloids is suggested on the basis of the easily obtainable quantities. In all of these cases, which are difficult for the conventional methods of density functional theory (DFT), MRSF shows results consistent with the experiment and the high-level ab initio computations. Hence, the present study documents the reliability and accuracy of MRSF and lays out the guidelines for its application to strongly correlated molecular systems.

Poster Presentation : **PHYS.P-193**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Emission Enhancements of Dyes with Dipole and Quadrupole Surface Plasmons of Composite Silver Nanosubstrates

Daedu Lee, GyoungHyun Song, Yoonsoo Pang*

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

Metal-enhanced fluorescence (MEF) has been recognized as a useful tool in biology, medical diagnostics, etc., due to largely increased emission signals and photostability of dyes. MEF of dyes results from the locally enlarged electric field and the plasmon-coupled emission of surface plasmon resonance (SPR) of metal nanoparticles. The dipole or quadrupole SPR of metal nanosurfaces has been used in the fluorescence enhancements of dyes, where the spectral overlap of the SPR bands with the dye's emission bands was considered the crucial factor for strong emission enhancements. However, the development of optimal metal nanosubstrates, including the dipole and quadrupole SPR bands of metal nanoparticles, has not been reported yet.In this study, composite silver colloidal films (SCFs) synthesized with the homogeneous silver nanoparticles of varying particle diameters were used to maximize the fluorescence intensity of dyes, where the emission bands of the dyes show good spectral overlaps with both the dipole SPR of one nanoparticle and the quadrupole SPR of the other nanoparticle. The emission enhancements and emission kinetics of the dyes have been measured by time-resolved fluorescence spectroscopy. In addition, strong fluorescence enhancements with the composite SCFs will be further understood by the finite-difference time-domain simulations on the local electric field enhancements around the silver nanoparticles.

Poster Presentation : **PHYS.P-194**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Excited-state aromaticity in dihydroazulene

Svetlana Shostak, Cheol Ho Choi[1,*]

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

Energy consumption is increasing continuously. Currently, gas and coil remain the main sources of thermal energy. However, its use results in several negative effects on our environment. Thus, one important challenge we facing now is to find alternative ways of obtaining and storing energy. Lately, photoswitching molecules have received great attention due to their high potential in many fields of science and technology, including the field of solar energy storage. Photoswitching molecules are capable of changing their properties upon photon absorption. Examples of such photoinduced reactions are photoinduced electron or proton transfer, bond rupture/formation, cis-trans isomerization.In our study, we investigate the photochemical reaction of dihydroazulene (DHA). Upon photoexcitation, this molecule undergoes an excited-state ring-opening resulting in the formation of cis-vinyleheptafulvene. Severe geometric difference between the initial compound and the one formed as the resresult of photoexcitation makes this molecule a particularly attractive subject to study. An interestingg aspect of the reaction is the effect of aromaticity on the reaction path. Using recently developed in our group mixed-reference spin-flip (MRSF) time-dependent density functional theory (TDDFT) we carried out nonadiabatic molecular dynamic (NAMD) as well as static calculations aimed to reveal the mechanism of the DHA ring-opening reation. NICS technique was applied to describe the role of excited and ground state aromaticity for this reaction.

Poster Presentation : **PHYS.P-195**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

RetroTRAE: retrosynthetic translation of atomic environments with Transformer

Umit Volkan Ucak, Juyong Lee[1,*]

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

Herein we present a new retrosynthesis prediction method, viz. RetroTRAE, which uses fragment-based tokenization combined with the Transformer architecture.RetroTRAE mimics chemical reasoning, and predicts reactant candidates by learning the changes of atomic environments associated with the chemical reaction.Atom environments stand as ideal, chemically meaningful building blocks, which together produce a high-resolution molecular representation. Describing a molecule with a set of atom environments establishes a clear relationship between translated product-reactant pairs due to the conservation of atoms in the reactions. Our model achieved a top-1 accuracy of 68.1% within the bioactively similar range for the USPTO test dataset, outperforming other state-of-the-art translation methods.Besides yielding a high level of overall accuracy, the proposed method solves the translation issues arising from the SMILES-based retrosynthesis planning methods effectively.Through careful inspection of reactant candidates, we demonstrated atom environments as promising descriptors for studying reaction route prediction and discovery.RetroTRAE provides fast and reliable retrosynthetic route planning for substances whose fragmentation patterns are revealed.Our methodology offers a novel way of devising a retrosynthetic planning model using fragmental and topological descriptors as natural inputs for chemical translation tasks.

Poster Presentation : **PHYS.P-196**

Physical Chemistry

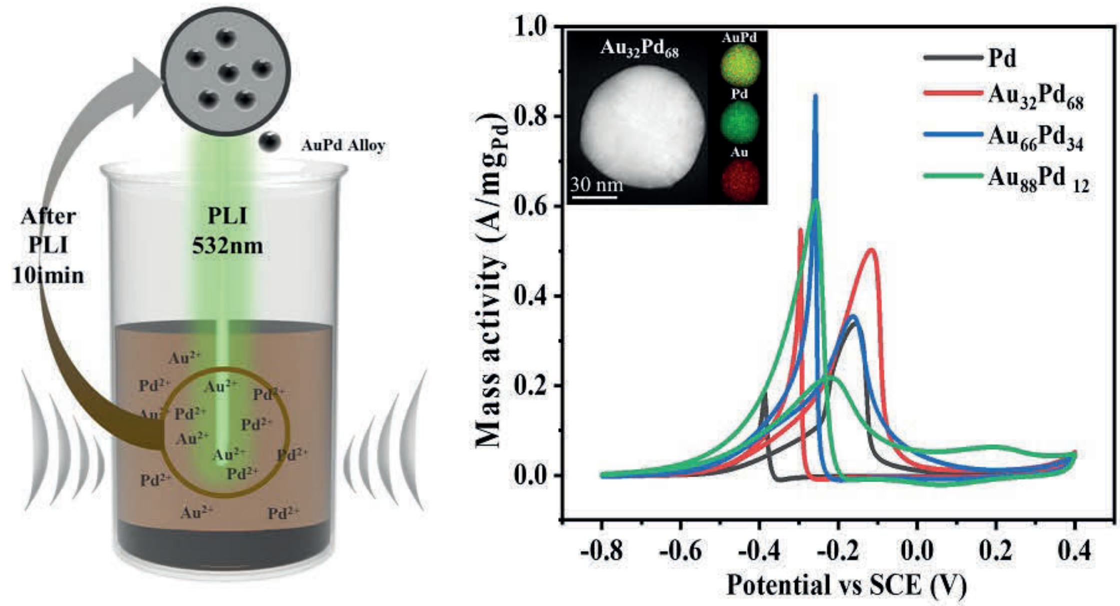
Exhibition Hall 1 THU 11:00~12:30

Insights into a Molar-Dependent Electrocatalytic Methanol Oxidation Reaction of Au-Pd alloy nanospheres synthesis by Pulsed laser irradiation

Sang Hun Yeon, Seung Jun Lee[1], Deviprasath Chinnadurai[2], Yiseul Yu, Young Wook Lee[3,*], Myong Yong Choi[1,*]

Gyeongsang National University, Korea
[1]*Department of Chemistry, Gyeongsang National University, Korea*
[2]*chemistry, Gyeongsang National University, Korea*
[3]*Department of Education Chemistry, Gyeongsang National University, Korea*

Direct methanol fuel cells have attracted extensive research interest because of their relatively high energy density and portability. CO poisoning effect and high cost of Pt induces the research for efficient non-Pt MOR electrocatalyst with higher CO tolerance. This report elaborates the modular designing and synthesize of molar ratio tuned Au–Pd alloy for the methanol oxidation reaction (MOR) by a one pot and extremely fast pulsed laser irradiation technique. The effective implementation of extremely rapid photoinduced reduction conditions resulted in the formation of well-dispersed and homogenous nanospheres of the Au–Pd alloy with uniform particle size. Improved electrocatalytic activity and CO tolerance attribute to Au alloying with Pd which enhances the charge transfer mechanism and reduced the CO binding strength. The optimized alloy (Au32Pd68) achieved relatively high mass and specific activities of 0.50 A/mgPd and 1.36 mA/cmPd2, respectively. Additionally, we studied the effect of the Au–Pd composition on the MOR activity and analyzed the reaction kinetics in depth. This work delivers the underpinning for implementing a laser-based technique to synthesize Pd-based alloy electrocatalysts for MOR application.


AuPd Alloy
After
PLI
10min
PLI
532nm
Au2+
Pd2+
Au32Pd68
AuPd
Pd
Au
30 nm
Pd
Au32Pd68
Au66Pd34
Au88Pd 12
Mass activity (A/mgPd)
1.0
0.8
0.6
0.4
0.2
0.0
-0.8
-0.6
-0.4
-0.2
0.0
0.2
0.4
Potential vs SCE (V)

Poster Presentation : **PHYS.P-197**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Li growth dynamics in Lithium metal battery by in situ liquid cell optical microscopy and transmission electron microscopy

Yonggoon Jeon, Jungwon Park*

School of chemical and biological engineering, Seoul National University, Korea

High energy density and cycling stability of lithium-ion batteries(LIBs) are receiving great attention as LIBs have been essential goods in our life from portable devices to electric vehicles(EVs). Therefore, understanding the dynamics of lithium dendrite and solid electrolyte interphase(SEI) formation is important to improve the performance and lifespan of LIBs. In this aspect, we observed the differences in reactivity, stability and morphological change in two types of electrolytes, carbonate (ethylene carbonate (EC) /diethyl carbonate (DEC)) and ether (1,3-dioxolane (DOL) / dimethyl ether (DME)) type using in situ liquid-cell transmission electron microscopy (LC-TEM) and optical microscopy(OM). Also, we investigated the plating and stripping dynamics depending on current density by in situ liquid cell OM. In addition, the dendritic growth of Li in different electrolyteenvironment were analyzed through in situ OM and LC-TEM. These results are expected to shed light on the understanding of Li dendrite growth in LIBs and rational design of the next-generation batteries.

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Poster Presentation : **PHYS.P-198**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Compound Identification in Electron-Ionization Mass Spectra via Neural Machine Translation.

Islambek Ashyrmamatov, Juyong Lee[1,*]

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

Determining the chemical composition of unknown compounds plays a central role in chemical analysis.Mass spectral reference libraries, as the collections of chemical structures and their spectra, provide a means of identification for compounds. However, existing libraries suffer from a coverage problem, which can be partially solved by in-silico spectra augmentation. Alternative to reference library matching, we propose a direct spectra-to-molecule translation approach for structure prediction for electron-ionization mass spectra. This is the first method using neural machine translation to identify an unknown molecule from its mass spectrum. We evaluated our method with NIST main library, and the results indicate that our novel framework presents an effective compound identification by using Transformer architecture. Our method can work cooperatively with database spectral matching to improve identification accuracy. This proposed approach has a high potential for broad applications in chemicthe al analysis of unknown substance.

Poster Presentation : **PHYS.P-199**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

The Study on SERS Spectral Changes of Reporter Molecules by Enzyme Reaction

Eungyeong Park, Hyejin Chang[1], Young Mee Jung[*]

Department of Chemistry, Kangwon National University, Korea
[1]*Division of science education, Kangwon National University, Korea*

Surface-enhanced Raman scattering (SERS) has been actively studied with a lot of advantages such as ultra-sensitivity, selectivity, and photostability. SERS spectrum reflects the changes in the polarizability and electronic density of molecules. In this study, we explore that the SERS spectrum of reporter molecules was changed by enzyme reaction between reporter-linked lactate oxidase (LOx) and lactate. Functionalized silver nanoparticles with LOx conjugated SERS reporter (4-mercaptobenzoic acid) were fabricated and used for the measurement of SERS spectra of lactate from10^{-4} M to 10^{-7} M.

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Poster Presentation : **PHYS.P-200**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Characterization of Multi-Stimuli Responsive P(NIPAAm-*co*-AAc) Hydrogel during the Heating and Cooling Processes

Minkyoung Kim, Yeonju Park[1], Young Mee Jung[*]

Department of Chemistry, Kangwon National University, Korea
[1]*Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*

Until now, polymer hydrogels whose volume and properties change due to various external environmental stimuli have been studied. Poly(*N*-isopropylacrylamide-*co*-acrylic acid) [P(NIPAAm-*co*-AAc)] hydrogel is a multi-stimuli responsive polymer that responds to various external stimuli such as temperature, pH and CO_2 gas. It shows sol-gel and volume phase transitions under specific temperature which is called lower critical solution temperature (LCST). PNIPAAm has an LCST near 32 °C in an aqueous system. LCST of PNIPAAm-*co*-AAc is higher than that of PNIPAAm. In this study, the phase transition temperature and mechanism of the pH/temperature-sensitive copolymer P(NIPAAm-*co*-AAc) hydrogel during the heating and cooling processes were investigated at various pHs using IR spectroscopy and two-dimensional correlation spectroscopy. The detail of the results will be discussed in this presentation.

Poster Presentation : **PHYS.P-201**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Effect of structure-mediated exciton transition behavior on SERS activity of layered structure of semiconductor

Shuang Guo, Sila Jin, Eungyeong Park, Chen Lei[1], Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea
[1]*College of chemistry, Jilin Normal University, China*

In recent years, semiconductors have been widely used in surface enhanced Raman scattering (SERS) substrates due to their unique properties, especially the interaction between semiconductors and adsorbed molecules, which has always been a research hotspot. In order to study this problem, we adopted a new type of MoS_2-Ag reduced graphene oxide (rGO) composite material as a SERS active substrate to investigate the effect of structure-mediated changes on SERS. The rGO nanosheets with Ag nanoparticles was worked as a platform to growth flower-like spherical MoS_2 to form a MoS_2-Ag-rGO composite based on a simple hydrothermal method. Studies shown that the structural-mediated changes of layered semiconductors can change the interlayer van der Waals interaction and exciton transition of MoS_2 compared to pure MoS_2under the same conditions. The effect of this structure-mediated change on SERS activity was studied using methylene blue as a probe molecule. The details of the mechanism of this structure-mediated change in SERS system will be discussed in this presentation.

Poster Presentation : **PHYS.P-202**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Rational design and photochemical characterization of novel fluorescent compound through computational study

Ji Hye Lee, Hyonseok Hwang[*]

Department of Chemistry, Kangwon National University, Korea

Most of the heterocycles possess important applications in various fields, including polymer chemistry, material science, and medicinal chemistry. In recent years, numerous studies have mainly focused on the application of such systems as organic fluorophores, since fused aromatic compounds have extensive conjugated π-systems and rigid planar structures, which are necessary conditions for fluorescence. In a study of 6-(thiophen-2yl) indolizino[3,2-c]quinolines (IQs) that are fluorescent compounds, the importance of a methoxycarbonyl (MC) group attached to the IQ scaffolds was suggested in the presence of a thiophene group. In this study, we designed novel IQs guided by density functional theory (DFT) calculations and explored the optical properties of the IQ derivatives together with fractional atomic orbital contribution (FAOC) analysis. To characterize the photophysical properties of substituted-IQs and understand the effect of the MC substituent in the absorption and emission spectra changes of IQ derivatives, the vertical excitation energies, oscillator strengths, and absorption wavelengths for the compounds were obtained via time-dependent (TD) DFT calculations. Comparisons with the experimental results verify the validity of the FAOC analysis, which can be used as a computational method to predict spectral shifts for fluorophores and to design novel fluorescent compound.

Poster Presentation : **PHYS.P-203**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Second-Harmonic Generation and Photoluminescence Imaging of Few-Layer Hexagonal Boron Nitride

Yeri Lee, Juseung Oh, Hyeon Suk Shin[1], Sunmin Ryu*

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

Hexagonal boron nitride (hBN) has recently attracted considerable attention for its nanophotonic applications in the UV region because of its wide bandgap (7.25 eV). However, the sizeable optical gap has hampered efficient structural characterizations of the dielectric material using conventional photoluminescence (PL) and Raman spectroscopy. In this study, we report on two correlated nonlinear optical imaging modes to characterize the structure of hBN: second-harmonic generation (SHG) and two-photon PL. Two types of few-layer hBN samples were prepared by mechanical exfoliation and chemical vapor deposition (CVD). SHG and PL signals generated with 140 fs pulses at NIR wavelength were simultaneously obtained with a CCD detector. CVD-grown hBN samples showed substantially weaker SHG but stronger visible PL signals than exfoliated ones. Polarized SHG imaging of CVD-hBN revealed spatial inhomogeneity and orientational disorder that could not be seen in exfoliated samples. The structural quality and differences of the two samples will be discussed in detail. 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.

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Poster Presentation : **PHYS.P-204**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Time-Resolved Emission and Reflectance Spectroscopy Study of Excitonic Behaviors in 2D $CrCl_3$

Hyesun Kim, Sunmin Ryu*

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

Two-dimensional chromium(III) chloride ($CrCl_3$) offers the opportunity for applications in various fields including optoelectronic devices and magnetic sensors because of its intrinsic magnetism down to monolayer limit and strong visible absorption of its bulk form. In this work, we studied the excitonic behaviors of few-layer to bulk $CrCl_3$. Absorption/photoluminescence (PL) spectroscopy and time-correlated single-photon counting (TCSPC) were used to elucidate its electronic structure and excitonic lifecycle, respectively. There was no significant spectral change with the number of layers in Raman, absorption, and PL signals. Surprisingly, however, the PL lifetime showed a drastic reduction from 1940 ns to 2 ns with decreasing thickness from 61 to 3 nm. The origins for the accelerated relaxation in 2D forms will be discussed based on the control experiments to address the effects of ambient instability and possible photoinduced reactions.

Poster Presentation : **PHYS.P-205**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Redox and Magnetic Properties of Organic Photoredox Catalysts in Excited States

Jiyoon Choi, Hyungjun Kim*

Department of Chemistry, Incheon National University, Korea

The photoredox catalysts(PCs) have contributed a lot to organic synthesis by using light to promote electrons to accelerate chemical reactions and enable new chemical reactions. Organic photoredox catalysts are currently being actively studied as alternatives to transition metal photoredox catalysts.In order to develop a new photoredox catalysts, it is important to grasp the redox properties of the photoredox catalysts in the ground state and the excited state. However, it is still unclear how to accurately implement the excited redox potential in a quantum chemistry simulation. Therefore, research to achieve highly accurate prediction for the redox properties of photoredox catalyst is of great importance. In this study, several factors were considered to predict the redox properties in the excited state with high accuracy for selected model systems of dihydroquinoxalino[2,3-b] quinoxaline derivatives : the magnetic properties of ground and excited states, the solvent medium effect on excited-state geometries, an adequate amount of Hartree–Fock exchange (HFX),[3] and the consideration of double-excitation character in excited states.[2] ,[4] We established a theoretical protocol based on spin flip density functional theory (SF-DFT) that could provide highly accurate estimations of photophysical properties and ground-/excited-state redox properties, focusing on the four factors mentioned above.[1] This theoretical protocol is expected to contribute to the efficient design of new promising PC candidates. References[1] J. Choi and H. Kim, J. Chem. Theory Comput. 2021, 17, 767−776.[2] D. Casanova and A. I. Krylov, Phys. Chem. Chem. Phys. 2020, 22, 4326−4342.[3] S. A. Mewes , F. Plasser , A. Krylov and A. Dreuw, J. Chem. Theory Comput. 2018, 14, 710−725.[4] Z. Rinkevicius , O. Vahtras and H. Årgen, J. Chem. Phys. 2010, 133, 114104.

Poster Presentation : **PHYS.P-206**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Intramolecular Charge Transfer of Michler’s Ketone Studied by Femtosecond Stimulated Raman Spectroscopy

Gisang Lee, Myungsam Jen, Taehyung Jang, Yoonsoo Pang*

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

Photo-induced intramolecular charge transfer (ICT) of dye molecules is of great interest in biology and chemistry fields for its wide applications to solar energy conversion, photovoltaics, and fluorescence sensing. Michler’s ketone (MK) is benzophenone’s derivative with two electron-donating dimethylamino groups attached to each end of both phenyl rings. According to density functional theory (DFT) simulations, the ground state structure of MK is totally symmetric with the plane of both phenyl rings are tilted about 50° to each other. Excited-state dynamics of MK depends largely on the solvent properties including polarity and hydrogen bonding, where the multiexponential decays of time-resolved absorption and emission signals of MK have been interpreted as the complicated dynamics including multiple ICT states. Flattening of the molecular structure of MK was proposed from time-dependent DFT simulations and further changes in the molecular structure such as the twist of dimethylamino group was suggested for the complicated ICT dynamics. However, experimental evidence of such structural changes during the ICT process has not been provided yet.In this study, the ICT dynamics of MK will be investigated by femtosecond stimulated Raman spectroscopy (FSRS), where vibrational coupling between the skeletal vibrations of νC=O and ν8a of phenyl rings may provide the key to the structural changes with the ICT dynamics. We also observed the twist of dimethylamino group in our recent FSRS works on several push-pull dyes. Thus, structural identities of MK during the ICT dynamics in the singlet excited states can be further confirmed by FSRS measurements between the multiple rotamers of dimethylaniline and dimethylamino groups.

Poster Presentation : **PHYS.P-207**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Structural Insights of Lactamase-like Esterase with *para*-Nitrophenyl Acetate (*p*NPA) and Nitrocefin (NCF): Molecular Dynamics Simulation Studies

Youhyun Nam, Rakwoo Chang[1,*]

University of Seoul, Korea

[1]Department of Applied Chemistry, University of Seoul, Korea

Penicillin-binding protein (PBP)/β-lactamase (βL) homologs from *Pseudomonas fluorescens* (PfEstA), *Ruegeria pomeroyi* (RpEstA), and *Caulobacter crescentus* (CcEstA) are esterases with class C β-lactamase activity. These enzymes have a two-step catalytic mechanism similar to class C β-lactamase: acylation and deacylation. In these enzymes, the catalytic triad is composed of serine (Ser), lysine (Lys), and tyrosine (Tyr). During the acylation step, Ser is known to act as a nucleophile and Lys and Tyr as general bases. But the exact mechanism is still unknown. To understand the relative activity of three esterases , we performed Molecular Dynamics (MD) simulation of these enzymes with two different ligands. One is *para*-Nitrophenyl acetate (*p*NPA), an ester and the other is Nitrocefin (NCF), which is well known as a β-lactam antibiotic. To examine how well the ligands and catalytic triad form the stable conformation for the nucleophilic attack, we calculated structural properties such as distance between the oxygen of serine and carbonyl carbon of the ligands, Bürgi-Duniz, and Flippin-Lodge angles. The interactions between the ligand and nearby amino acids including hydrogen bonds and π- π interactions were also considered. According to the corresponding experimental results, RpEstA with both *p*NPA and NCF has significant activity compared to the others. The properties calculated from simulation results also showed the noticeable differences between RpEstA and the others. These showed that the structural results with MD simulation can be used for the studies of the catalytic mechanism of the esterase.

Poster Presentation : **PHYS.P-208**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Intramolecular Charge Transfer Dynamics of Anthraquinone Derivatives Confined in the Reverse Micelles

Taehyung Jang, Gisang Lee, Yoonsoo Pang*

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

Excited-state intramolecular charge transfer (ICT) of chromophores has been extensively studied experimentally and theoretically for applications to solar energy conversion, photovoltaics, fluorescence sensing, etc. 1-Aminoanthraquinone (AAQ) shows ultrafast (150-180 fs) ICT dynamics in the excited state with the internal rotation of the amino (-NH_2) group attached to the anthraquinone backbone in our recent femtosecond stimulated Raman spectroscopy (FSRS) measurements. The major vibrational modes of AAQ, including νC-N + δCH at 1200-1230 cm^{-1} and νC=O at 1300-1330 cm^{-1}, represent the structural changes of ICT dynamics, which is also strongly coupled to the low frequency vibrational modes including the intermolecular hydrogen bonding with the surrounding solvent molecules of dimethyl sulfoxide.In this research, the excited-state dynamics of AAQ and its derivative, 1-methylaminoanthraquinone, in the confined environment of reverse micelles are investigated by time-resolved electronic and vibrational spectroscopy. Since the solvent properties of the nanopools of the reverse micelles, such as the solvent polarity or viscosity, appear distinct from the bulk, the ICT dynamics of anthraquinone derivatives with the rotation of amino or methylamino groups are expected to slow down in the reverse micelles. Furthermore, the photophysical properties of these anthraquinone dyes in the reverse micelles, including the Stokes shifts, quantum yields, and nonradiative decay rates, depending on the size of nanopools or the surfactant charges, will also be investigated by steady-state and time-resolved fluorescence measurements.

Poster Presentation : **PHYS.P-209**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synergic effects of the surface hardening agent and cement materials on photocatalytic activity of Fe-loaded TiO_2 particles towards NO oxidation

Hyun Ook Seo*, **Young Dok Kim**[1,*]

Department of Chemistry and Energy Engineering, Sangmyung University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Two Fe-loaded TiO_2 particles (Fe-P25 and Fe-R996) were prepared via temperature regulated chemical vapor deposition (tr-CVD) of Fe-oxide on two commercial TiO_2 particles (P25 and R996) and subsequent thermal annealing. Photocatalytic NO oxidation was performed under the conditions of 50RH% and visible light irradiation using a flow-type reactor in the presence of two modified particles (Fe-P25 and Fe-R996). Each particle was mounted in the reactor after either drop-casted on a stainless-steel plate or spread on a cement block using a commercial surface hardening agent as a binder. The Fe-R996 outperformed the Fe-P25 in terms of NO removal, NO_2, and NO_3^- evolutions when they were spread on cement blocks using the SHA, although the drop-casted Fe-R996 exhibited much lower activity than the drop-casted Fe-P25. It indicated the existence of the synergic effects of the SHA and cement materials on the photocatalytic activity of Fe-loaded TiO_2 particles, which depends on the intrinsic structure of Fe-loaded TiO_2 particles. The additional surface analysis using XPS and FT-IR implied the facilitation of the NO_3^- diffusion from the top surface into the deeper parts of the photocatalytic layers on cement blocks by mixing with the SHA. Our experimental observations indicate that the combination of photocatalytic particles with other agents, such as SHA, during the immobilization process can also affect their photocatalytic activities. We believe that this has large implications for the application of photocatalysts in building and construction sites.

Poster Presentation : **PHYS.P-210**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Iridium doped electrospun $Co_3V_2O_8$ nanofibers and their electrochemical properties

Song Hee Lee, Dasol Jin, Chongmok Lee*, Myung Hwa Kim[1,*]

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

We report the facile synthetic methodology of $Co_3V_2O_8$ nanofibers doped with Ir metal via a simple electrospinning process followed by the thermal annealing. The well-defined fabric nanostructures are then characterized by scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), X-ray diffraction (XRD) and transmission electron microscopy (TEM). $Co_3V_2O_8$ nanofibers generate sensing performance for detecting AA(L-ascorbic acid). By controlling the weight percent of the Ir, furthermore, the prepared nanofiber composite $Co_3V_2O_8$/ Ir exhibits greatly enhanced electrochemical performances. The synthesized $Co_3V_2O_8$ nanofibers doped with Ir metal represent the significantly enhanced OER activity in alkaline solution and the sensing performance for sensitively detecting AP(4-acetamidophenol) compared to single $Co_3V_2O_8$ nanofibers. We also report that the OER catalytic performamces of the nanofiber composite $Co_3V_2O_8$/ Ir can be comparable to Pt catalyst.

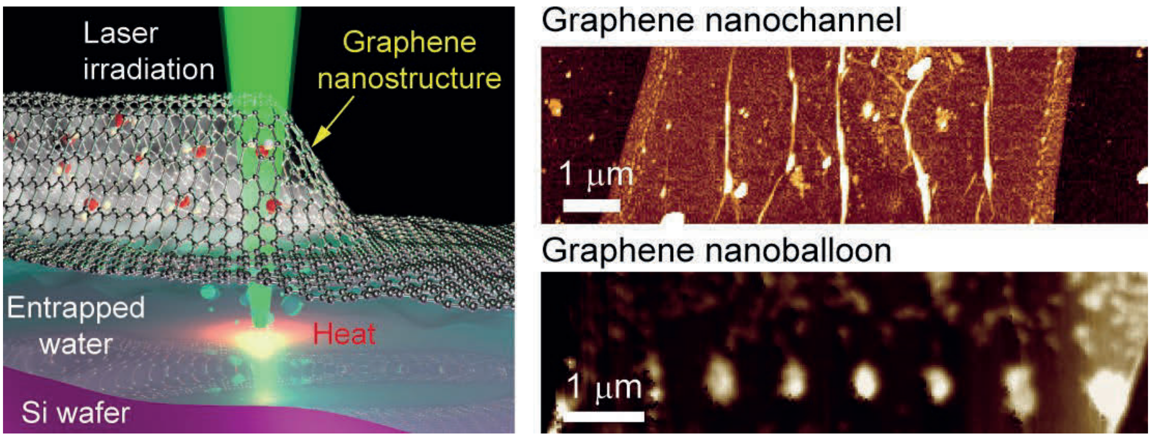
Poster Presentation : **PHYS.P-211**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Formation of Graphene Nanochannel and Nanoballoon using Laser Induced Vaporization of Entrapped Water

Jehyun Oh, Minsuk Park, Sungmin Bong, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

Graphene has excellent mechanical strength, transparency, and flexibility and has a potential for one atomic thick nanostructure. Constructing graphene as a nano building block is important for the miniaturized functional nanodevices.In this poster, we found that graphene nanostructures including graphene nanochannel and nanoballoon are realized by irradiating graphene-entrapped water-hydrophobic substrate by focused laser. For this, a monolayer graphene was mechanically exfoliated on a hydrophobically functionalized silicon substrate. Entrapped water was achieved by immersion of graphene/the sample into water from few to few tens days. Laser irradiation of the sandwiched sample creates graphene nanochannel and nanoballoon, depending on continuity of laser writing. Atomic force microscope (AFM) measurement shows that the graphene nanostructure has few hundreds nanometer in width and few tens nanometer in heights. Especially, upon closer look, the result shows that the formation of graphene nanochannel is accompanied by lateral shrinkage. The suggested mechanism for the formation of the nanostructure is the initial water entrapment, followed by bulging up of graphene by entrapped water vaporization *via* laser absorption. The optical change of graphene created by entrapped water was monitored by a series of Raman mapping in which water entrapping results in strain- and doping-relieved graphene states by showing progressive red shift of the G and 2D bands, indicative of weakened interaction between graphene/substrate. Controlled formation of graphene nanostructures using laser will be a vehicle for graphene to be utilized for various applications such as bio sensing, ion transport, and water filtration.


Laser irradiation
Graphene nanostructure
Entrapped water
Heat
Si wafer
Graphene nanochannel
1 μm
Graphene nanoballoon
1 μm

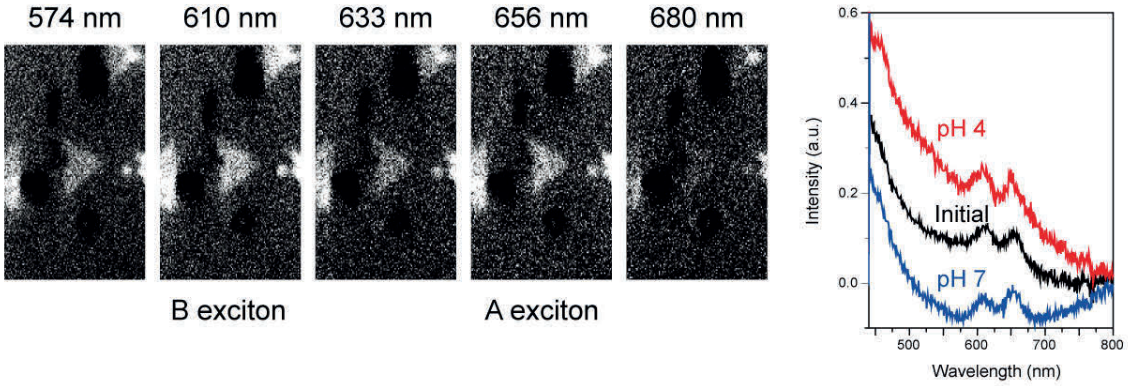
Poster Presentation : **PHYS.P-212**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

pH-Dependent Optical Properties of Chemical Vapor Deposition-Grown MoS_2 *via* Reflection Imaging

Sungmin Bong, Sang-Yong Ju[*]

Department of Chemistry, Yonsei University, Korea

Molybdenum disulfide (MoS_2) is a few atomic thick two-dimensional material which possesses semiconducting property with band gap. Defect-free semiconducting MoS_2 is potentially serves as optoelectronic semiconductor having high current on/off ratio semiconductors and high quantum efficiency. However, the study on MoS_2 doping is still limited, hampering further applications.In this poster, we report the optical properties of chemical vapor deposition (CVD)-grown MoS_2 according to pH control *via* reflection imaging. Initially, MoS_2 was synthesized on a Si substrate using two precursors of sulfur and MoO_3 by using CVD method. The synthesized MoS_2 was transferred to transparent glass substrates *via* dimethyl sulfoxide assisted poly(dimethylsiloxane) stamping method. The samples were subjected to pH-controlled viewport chamber which allows to probe reflection image of MoS_2 through a coverslip. Initially, reflection image spectroscopy collects a series of as-prepared MoS_2 image which shows 610 nm and 656 nm brightness corresponding to B and A excitons. Upon immersion of the sample in different pH buffer, reflection spectra of MoS_2 displays gradual increases in A and B excitons as decreasing pH. Subsequent Raman and photoluminescence (PL) behaviors were also acquired and showed similar behavior. This study will provide the underlying mechanism on how absorption and PL behaviors are linked in few atomic thick MoS_2.


574 nm
610 nm
633 nm
656 nm
680 nm
B exciton
A exciton
Intensity (a.u.)
0.6
0.4
0.2
0.0
pH 4
Initial
pH 7
500
600
700
800
Wavelength (nm)

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **PHYS.P-213**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

The electrochemical properties of electrospun CaRuO3 nanofibers synthesized by electrospinning method

Seokin Yun, Yoonkyeong Kim, Myung Hwa Kim[1,*], Youngmi Lee[1,*]

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

We report a facile synthesis for the crystalline perovskite nanostructure of calcium ruthenium oxide(CaRuO3) by using the electrospinning process followed by the thermal annealling. The morphology, the crystal structure and the elements ratio of prepared crystalline electrospun CaRuO3 nanofibers were carefully characterized by Field Emission Scanning Electron Microscope(FE-SEM), Energy Dispersive Spectroscope(EDS), Transmission Electron Microscope(TEM), X-ray Diffraction(XRD), and Raman Spectroscopy. We have investigated the electrochemical performance for CaRuO3 nanofibers as a OER catalyst in acidic and basic solution, resulting in the better performance than commercial Ir. Furthermore, electrospun CaRuO3 nanofibers represents a good sensing behavior for detecting ascorbic acid(AA) with high selectivity and sensitivity.

Poster Presentation : **PHYS.P-214**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Synthesis of Iridium diphosphide(IrP_2) nanoparticles and its application for Amperometric Sensing of H_2S

Seoyoung Jeong, Youngmi Lee[*], Myung Hwa Kim[1,*]

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

In our study, we synthesized Iridium diphosphide(IrP_2) nanoparticles by simple participation and phosphorization methods. Although most of reported Iridium diphosphide are synthesized at high pressure and high temperature, we successfully prepared IrP_2 nanoparticles at relatively low temperature(650℃). The morphology and structure of prepared IrP_2 nanoparticles were carefully characterized by SEM(Scanning Electron Microscopy), EDX(Energy Dispersive X-ray spectroscopy), XRD(X-ray Diffraction), TEM(Transmission Electron Microscopy), XPS(X-ray Photoelectron Spectroscopy). The results indicated that 20-50nm sized nanoparticles are synthesized successfully. Moreover, it shows high amperometric sensing performance for Hydrogen sulfide (H_2S) gas. It is well-known that Iridium-based nanomaterials has their intrinsic merits of high activity, conductivity and durability, so it has been widely stuided for various electrochemical reactions such as OER, HER, ORR, carbon dioxide reduction reaction, etc. Besides, transition metal phosphides (TMPs) have been regarded as promising alternative to replace Pt-based materials with high activity and stability. Thus, we can further investigate the electrocatalytic activities for the hydrogen evolution reaction and improved electroactivity for H_2S gas sensing.

Poster Presentation : **PHYS.P-215**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Alignment of symmetric top molecules by photoexcitation with linearly and circularly polarized light

Kamal Mishra, Changseop Jeong, Ji Yeon Yun, Jiyoung Heo[1,*], Nam Joon Kim[*]

Department of Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Green Chemical Engineering, Sangmyung University, Korea*

In this work, we have explained the experimentally observed band features in the vibrational difference spectra as well as high-resolution electronic difference spectra of the three most stable conformers of (-)-pseudoephedrine. The difference spectra were obtained by the difference of R2PI ion signal obtained by linearly (LP) and circularly polarized (CP) lights. We observed that the P and R-branch transitions show positive signs whereas the Q-branch transition shows the negative sign in the LP-CP difference spectra for all the conformers. The observation of different spectral features for P, Q and R-branch transitions is explained based on the difference in the M distribution created by the linearly polarized light and the circularly polarized light where M is the projection of the total angular momentum (J) on the space fixed Z-axis. Our theoretical analysis suggests that the linearly polarized (LP) light creates a larger anisotropic M-distribution than the circularly polarized (CP) light for P and R-branch transitions hence the LP-CP anisotropic M distribution is positive. For Q-branch transition, the circularly polarized (CP) light creates more anisotropic M distribution than the linearly polarized (LP) light, hence the LP-CP anisotropic M distribution is negative.

Poster Presentation : **PHYS.P-216**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Electrospun $SrIrO_3$ nanofibers as highly stable pH universal OER catalyst

Minju Kim, Seungsun Shin, Youngmi Lee*, Myung Hwa Kim*

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

We report the synthesis of electrospun $SrIrO_3$ nanofibers and its application in Oxygen Evolution Reaction (OER) under the broad range of pH condition. We synthesized the perovskite $SrIrO_3$ nanofibers by using electrospinning method followed by the thermal annealing process. We carefully controlled the morphology and crystallinity mainly through the growth temperature, time, and composition of the precursor solution. The prepared nanofibers were thoroughly investigated by scanning electron microscopy (SEM), transmission electron microscopy (TEM), inductively coupled plasma-mass spectrometer (ICP-MS) and X-ray diffractometer (XRD). Perovskite structure has been recently attracting attention for its high OER performance. Previously synthesized $SrIrO_3$ showed that Sr was leached during the test and IrO_3 or anatase IrO_2 motifs was formed on the surface, which resulted in gradual improvement in OER performance over time in acidic solution. However, $SrIrO_3$ we report here shows high performance without change over time. It also shows higher performance than commercial IrO_2 catalyst in all acidic, neutral, and alkaline solutions. In addition, the change in voltage was very small during the 20000 second test of the chronopotentiometry, showing the high stability in all the previously mentioned solutions. the morphology of nanofibers was also maintained even after the test time interval.References[1] Seitz, L. C.; Dickens, C. F.; Nishio, K.; Hikita, Y.; Montoya, J.; Doyle, A.; Kir, C.; Vojvodic A.; Hwang, H. Y.; Norskov, J. K.; Jaramillo, T. F., A highly active and stable $IrO_x/SrIrO_3$ catalyst for the oxygen evolution reaction. Science, 2016, 353, 1011–1014.

Poster Presentation : **PHYS.P-217**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

ZnV2O6 and CrVO4 nanostructures driven by a simple acid-base reaction with the thermal annealing process

Kyungmin Kim, Myung Hwa Kim[1,*]

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

Vandium oxide, a semiconductor metal oxide, is widely used as a sensor. In this work, we incorporated Zn and Cr to vandium oxide crystal lattices to synthesize ZnV2O6 and CrVO4 alloy type metal oxides through a simple acid-base reaction followed by the heat treatment at high temperature. Zn and Cr, known as earth-abundant-metals, can readily improve the physicochemical performance by changing the bandgap of the existing vanadium oxide. We investigated the shape and structure of ZnV2O6 and CrVO4 by using Field Emission Scanning Electron Microscopy (FE-SEM), Energy Dispersive Sepctroscopy (EDS), X-ray diffraction (XRD) and Raman Spectroscopy. The electrical properties of the synthesized ZnV2O6 and CrVO4 are carefully tested in order to utilize for real applications.

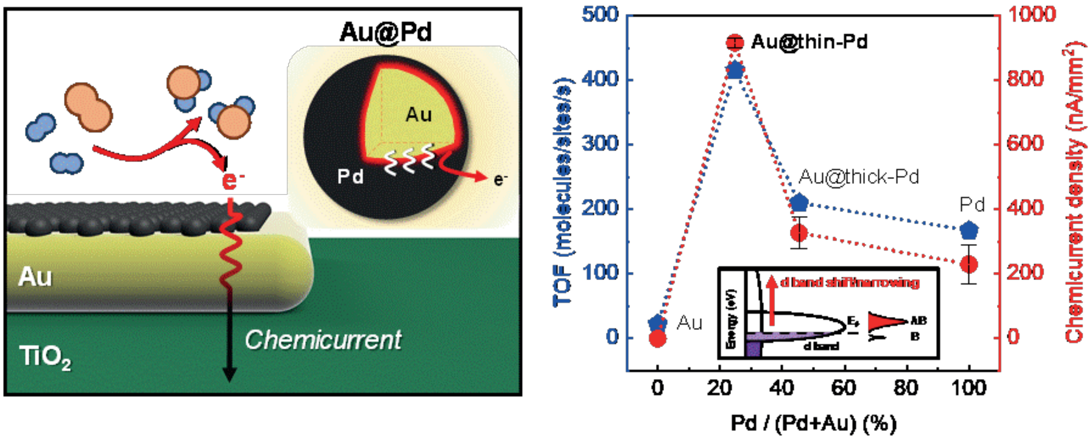
Poster Presentation : **PHYS.P-218**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Direct Observation of Electron Coupling Effect with Monitoring Hot Electron Behavior on Au@Pd Core-Shell Nanocatalysts

Beomjoon Jeon, Jeong Young Park[1,*]

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

Bimetal was introduced as a part of the research to find the optimal catalyst from an economic point of view considering the cost aspect of Pt, which is the best catalyst. The researchers have believed that the superior performance of the bimetal was due to the surface modification following the alloying process. As the surface is modified, the electronic behavior of the nanocatalyst can be controlled, and in this process, it is expected that the bimetal will exhibit an excellent performance. Therefore, the correlation between the electronic behaviors and the catalytic performances was confirmed through the study of directly detecting the hot electrons generated inside the nanocatalyst. Au@Pd core-shell nanoparticles were used as an experimental model because the interference effect on the reactivity of the bimetallic interface can be observed by controlling the thickness of the shell made of Pd as a catalyst. It was confirmed that the catalyst performance improved as the d-band of Pd increased under the influence of internal Au. In particular, by measuring the hot electrons generated during the reaction, it was shown that the hot electron flow of the catalyst having a thin shell was measured to be high, and even high as the ratio of the detected hot electron flow per unit catalytic reaction. Through this, it can be argued that the electron instability due to the movement of the d-band leads to the improvement of the catalyst performance, suggesting that this phenomenon can be observed through the hot electron detection method.


Au@Pd
Au
Pd
e-
e-
Au
TiO2
Chemicurrent
500
400
300
200
100
0
1000
800
600
400
200
0
TOF (molecules/sites/s)
Chemicurrent density (nA/mm2)
Au@thin-Pd
Au@thick-Pd
Pd
Au
d band shift/narrowing
Energy (eV)
EF
AB
B
d band
0
20
40
60
80
100
Pd / (Pd+Au) (%)

Poster Presentation : **PHYS.P-219**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Single-molecule Stimulated Raman Excited Fluorescence Spectroscopy of Visible Dyes

Jaeyoon Lee, Sang-Hee Shim*

Department of Chemistry, Korea University, Korea

Stimulated Raman excited fluorescence (SREF), a new hybrid spectroscopy that combines vibration characteristics of Raman spectroscopy with excellent sensitivity of fluorescence spectroscopy, demonstrated far-field single-molecule vibrational spectroscopy for the first time. However, the single-molecule signal is much lower than typical signal from directly excited fluorophores due to the low quantum yield of infrared fluorophores commonly used in SREF. SREF of visible dyes are limited by the lack of proper light source. In this study, we use two optical parametric oscillators (OPOs) synchronously pumped by a common pump source at 1031.2 nm for SREF of visible dyes. This laser system can generate two independently tunable pulses in 640-1150nm 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. ATTO665 with quantum yield of 0.6 is explored for SREF in the visible domain. We explore the wavelength-dependence of SREF signal of ATTO665 through theoretical modeling as well as spectroscopy measurement. We anticipate that our new scheme for SREF of visible dyes significantly increases the sensitivity to make single-molecule vibrational spectroscopy as a practical means for overcoming the spectral limit of single-molecule fluorescence spectroscopy.

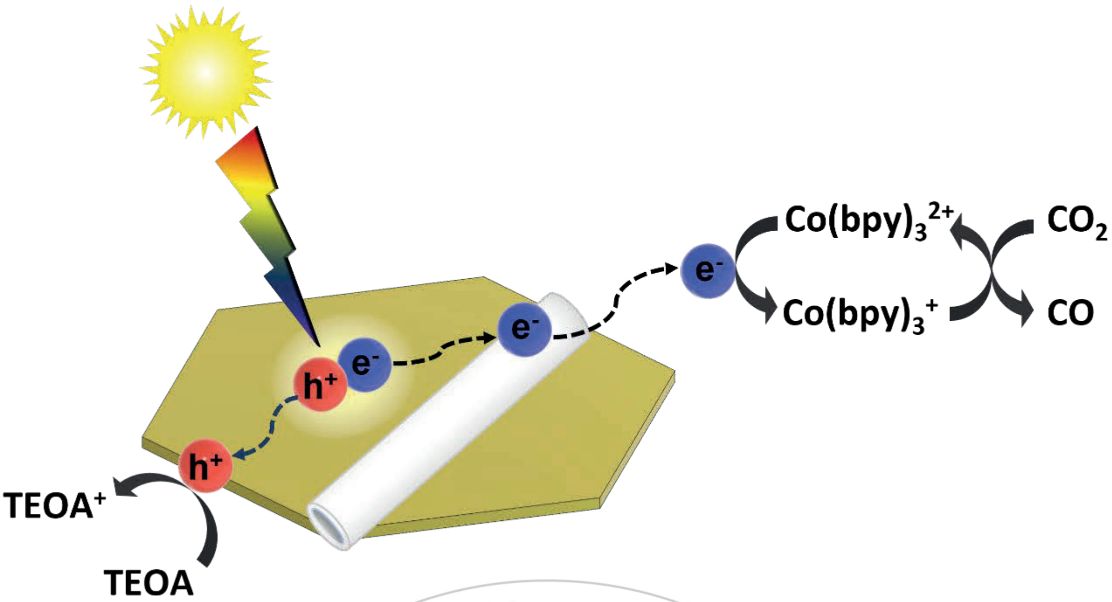
Poster Presentation : **PHYS.P-220**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Construction of 1D TiO_2 nanotube on ultrathin 2D $ZnIn_2S_2$ nanosheets Heterostructure for Photocatalytic CO_2 Reduction

Kim Eunhyo, Praveen Kumar Dharani[1], Hoang Khai Do[1], Putta Rangappa[2], Amaranatha Reddy[3], Tae Kyu Kim[1,*]

chemistry, Yonsei University, Korea
[1]*Department of Chemistry, Yonsei University, Korea*
[2]*Chemistry, Yonsei University, Korea*
[3]*Chemistry, INDIAN INSTITUTE OF INFORMATION TECHNOLOGY, India*

For the past few years, TiO_2 and $ZnIn_2S_4$ have been studied for conversion of CO_2 to generate environmentally friendly chemical energy under solar light. However, there was a restraint because of its poor CO_2 adsorption and charge carrying ability. In this study, TiO_2 nanotube (TNT) is fabricated as TiO_2 nanotube has higher electron mobility and specific surface area. Moreover, it has a wider bandgap around 3.5 eV that reduces recombination of electron-hole pair. To make a further improvement of electron delivery, $Co(bpy)_3^{2+}$ cocatalyst is introduced as it can capture electrons from ZIS conduction band to reduce CO_2. ZIS@TNT composite heterostructure is proved by Mott Schottky measurement and Diffuse reflectance spectroscopy. In this mechanism, photogenerated electrons in the ZIS conduction band are moving to the TNT conduction band, transferred to $Co(bpy)_3^{2+}$. This is reduced to $Co(bpy)_2$+ in turn, which can reduce CO_2 to CO . The optimized ratio of ZIS@TNT (10 wt%) has radically higher CO production than TNT and ZIS themselves. It produces CO with the rate of 4.37 mmol/(g·h), which is 2.6 times faster than that of ZIS. The stability of this material is proved by the long-time photocatalytic reaction. CO production and H_2 production were still continued for 70 hours and more, indicating that ZIS@TNT heterostructure has fine duration under solar light irradiation. This was also shown by 4 times of recycling test, showing almost same activity and selectivity during this experiment.


Co(bpy)$_3^{2+}$
CO$_2$
e$^-$
Co(bpy)$_3^{+}$
CO
e$^-$
e$^-$
h$^+$
h$^+$
TEOA$^+$
TEOA

Poster Presentation : **PHYS.P-221**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Multiphoton photofragmentation dynamics of cis and trans isomers of 1,2-dibromoethylene

Junggil Kim, Sang Kyu Kim*

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

Multiphoton photofragmentation dynamics of the cis and trans isomer of 1,2-dibromoethylene (1,2-DBE) has been investigated by photofragment excitation (PHOFEX) spectroscopy and velocity map ion imaging (VMI) using the picosecond laser pulse. Each conformational isomers of 1,2-DBE could be selectively excited using the distinct Rydberg transitions via two-photon excitation, and the unimolecular photofragmentation occurs very efficiently on the cationic excited state manifolds within the same laser pulse. It has been found that cis and trans isomers prefers different unimolecular photofragmentation pathways. For instance, the Br2+ product ion preferentially originates from the cis isomer rather than trans, on the other hand, fast and anisotropic Br+ ion is likely from the trans conformer. The highly anisotropic (β ~ 2) Br+ distribution could be attributed to the most probable D4 – D0 transition of the trans isomer where the transition dipole moment is parallel to the C-Br bond stretching coordinate. Similarly, the anisotropic (β ~ -0.5) distribution of Br2+ molecular ion well matches to the D4 – D0 transition of the cis conformer as the transition dipole moment is parallel to the C=C bond axis. The product state distributions have been interpreted with the aid of ab initio calculations.

Poster Presentation : **PHYS.P-222**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Novel quasi-exact solution for Michaelis-Menten kinetics

Kyungwoo Kim, Jaeyoung Sung[*]

Department of Chemistry, Chung-Ang University, Korea

Michaelis-Menten (MM) enzyme kinetics has been widely used for long times. However, the conventional enzyme kinetics is not accurate whenever substrate is not in excess or whenever the steady-state approximation does not hold. The steady-state approximation gets worse as enzyme concentration exceeds its substrate concentration, which is the case in many biological processes including viral infection, immune response, drug metabolism and so on. Here, we present a novel, quasi-exact solution of the standard enzyme kinetic equations, which provides the time profiles of substrate, enzyme-substrate complex and product concentrations at all times. Our solution is more accurate than the previously reported theories. We discover a new relationship between the enzyme reaction time (or the enzyme reaction rate) and enzyme concentration. We demonstrate our theoretical results for the β-galactosidase reaction.

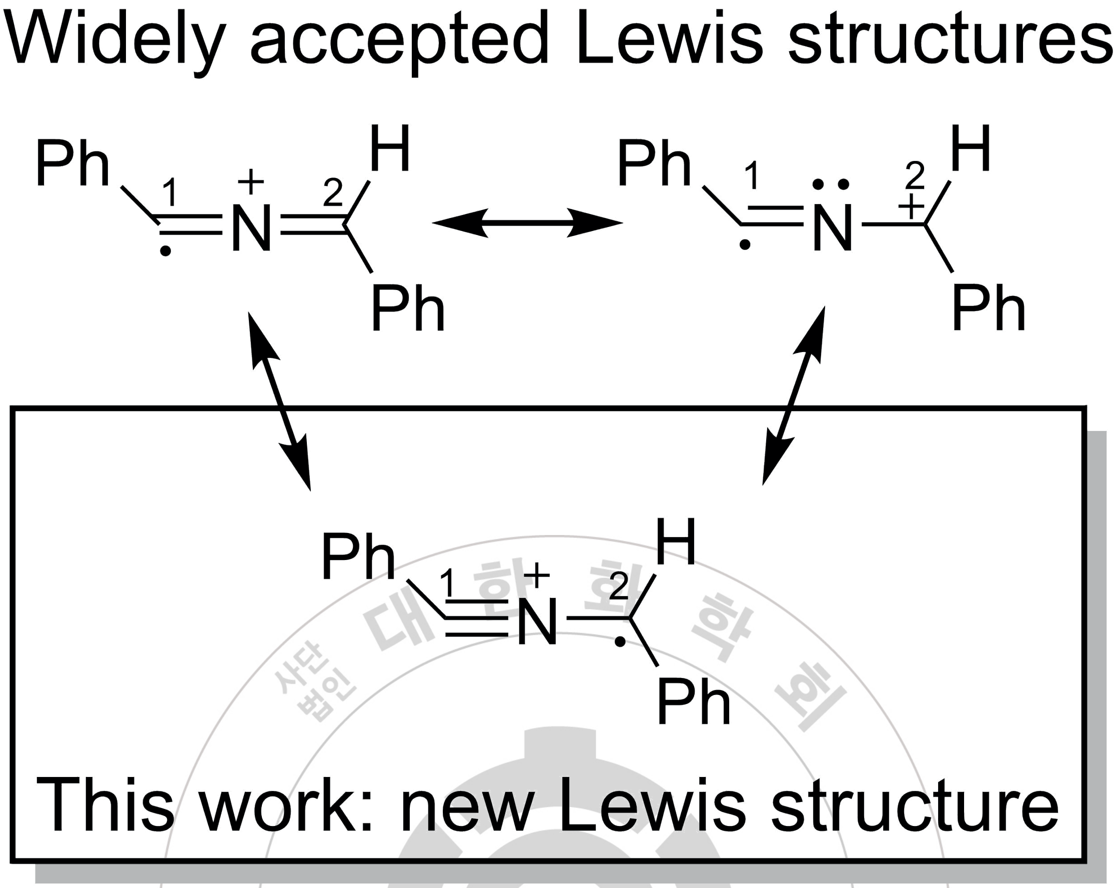
Poster Presentation : **PHYS.P-223**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Electronic structure of 2-azaallenyl radical cation

Daniel Yim, Hyungjun Kim*

Department of Chemistry, Incheon National University, Korea

2-Azaallenyl radical cation is a key intermediate observed during a number of [3+2]-cycloadditions utilizing 2H-azirine. Despite the importance of this key intermediate, there is no theoretical characterization of this radical partially due to the difficulty in the description of radical cations. Electronic structures of 1,3-diphenyl-2-azaallenyl radical cation and a variety of derivatives are investigated by high-level ab initio quantum chemical simulations to obtain deeper chemical insight for this intriguing radicals.In addition to a widely accepted Lewis structure of 1,3-diphenyl-2-azaallenyl radical cation, we suggest a new Lewis structure based on high-level ab initio calculations. Quadratic configuration interaction with single- and double-excitation (QCISD) gives spin population data of 1,3-diphenyl-2-azaallenyl radical cation having an unpaired electron delocalized over two carbon atoms adjacent to the central nitrogen atom. The second-order Møller–Plesset perturbation theory (MP2) with charges from electrostatic potentials using a grid-based method (CHELPG) scheme shows that the positive charge mainly resides on the on the central nitrogen atom of 1,3-diphenyl-2-azaallenyl radical cation, rather than the adjacent carbons as widely perceived. Alongside these electronic structures, we present a molecular geometry feature to support the new model.The new Lewis structure is in resonance with the widely accepted one, but the specific location of the unpaired electron is different from those. This study shows that the reaction mechanism which was believed to occur through pure radical addition needs to be reconsidered and revised. We will discuss this aspect in the future work.


Widely accepted Lewis structures
Ph
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This work: new Lewis structure

Poster Presentation : **PHYS.P-224**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

In-Situ Visualization of Surface Plasmon-Driven Hot Carrier Generation With Photoconductive AFM

Hyunhwa Lee, Jeong Young Park[1,*]

Center for Nanomaterials and Chemical Reactions, Institute for Basic Science, Korea
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Understanding the inter-coupling between surface plasmon and the electronic distribution in metallic nanostructures is a challenging topic to develop applications of plasmonic solar-cells and efficient photodetectors. Non-radiative surface plasmon decay produces highly energetic electron-hole pairs on the metal surface with desirable characteristics.[1] Since these carriers, called hot electron/or hot hole, dissipate their energies within the femtosecond resolution, it is hard to directly observe the fast-delivering during photocatalytic reaction. Thus, research on identifying surface plasmon-driven hot carrier dynamics at the nanoscale is of great importance. Here, we demonstrate the direct observation of surface plasmon-driven hot carriers created in a Schottky platform using photoconductive atomic force microscopy (pc-AFM).[2-3] We fabricated Au nanoprism on n-type TiO_2 film and p-type GaN substrate for detection surface plasmon-driven hot electron and hot holes, respectively. We show significant enhancement of photocurrent in the plasmonic platforms under light irradiation, providing direct evidence of plasmonic hot carrier generation. Experimental and numerical analysis verified that a confined |E|-field surrounding a single Au nanoprism spurred resonant coupling between localized surface plasmon resonance (LSPR) and surface charges, thus boosting hot carrier generation. Furthermore, geometrical and size dependence on the extraction of LSPR-driven hot carriers suggests an optimized pathway for their efficient utilization. The direct visualization of hot carrier flow at the nanoscale provides significant opportunities for harnessing the underlying nature and potential of plasmonic hot carriers.[Reference][1] I. Mondal, H. Lee, H. Kim, and J. Y. Park*, Adv. Funct. Mater. 30 (2020)[2] H. Lee, H. Lee, and J. Y. Park*, Nano Lett. 19 (2019)[3] H. Lee, K. Song, M. Lee*, and J. Y. Park*, Adv. Sci. 7 (2020)

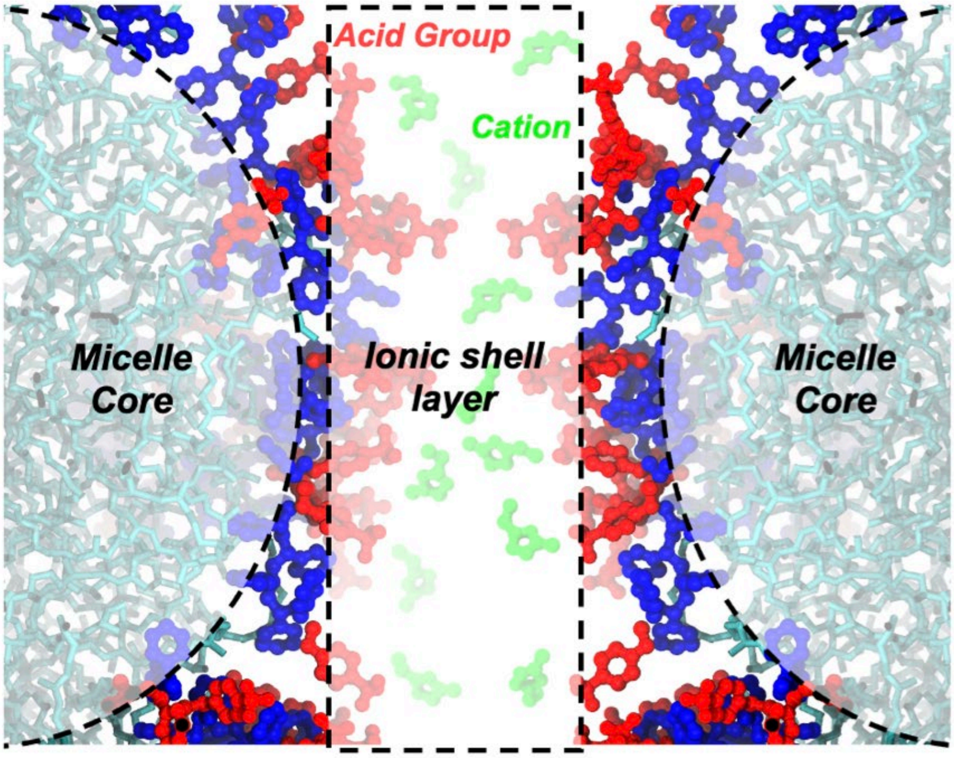
Poster Presentation : **PHYS.P-225**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

The stabilization mechanism of self-assembled low symmetry structure in charged block copolymer comprising ionic liquids

Seung Won Jeong, Chang yun Son*

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

To optimize the polymer electrolyte performance, the molecular understanding for the highly charged, microphase-separated electrolyte system is required. In this work, molecular dynamics (MD) simulations were performed to understand the role of electrostatic interaction at the interfacial layer in stabilizing different morphologies of charged polymer system. MD simulation revealed the micelles in a low symmetry cubic phase (A15) were closely contacted and made thin ionic shell layers at the interface. Moreover, a difference in the ion dynamics was observed between bulk and interfacial area due to electrostatic interactions between polymer and cation, resulting in morphology-specific ion dynamics. This work provides the mechanistic understanding of the electrostatic control of stability and ion dynamics in PEs with different morphologies and establishes a prospective avenue for advanced PEs with high ionic conductivity.


Acid Group
Cation
Micelle Core
Ionic shell layer
Micelle Core

Poster Presentation : **PHYS.P-226**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Molecular Evidence for the Formation of Real Active Metalloporphyrin-based Au Catalyst Revealed with Electrochemical Scanning Tunneling Microscopy

Yongman Kim, Jeong Young Park[1,*]

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

Developing efficient molecular catalysts, especially for the oxygen evolution reaction (OER), is essential in energy conversion devices. As a promising molecular catalyst, metalloporphyrins have been studied as a good model system; however, the relation to its structural stability and catalytic activity is still not fully understood because of their complexity. Thus, we exploit electrochemical scanning tunneling microscopy (EC-STM) as a powerful real-space imaging technique to unravel the morphological evolution of the 2,3,7,8,12,13,17,18-Octaethyl-21H,23H-porphine manganese (II) (MnOEP)/Au(111) interface during the electrocatalytic reaction process. Notably, in alkaline solution, the catalytic performance is significantly increase after the first potential sweep, directly related to the formation of the MnO_x–porphyrin complexes, driven by an irreversible oxidation-reduction process. In situ EC-STM has revealed (1) the oxidized MnOEP phases (MnOEP–OH^- or MnOEP–O_x) at the anodic branch as a protrusion, (2) the massive oxidation of MnOEP and the rapid decomposition as the disordered structures, and (3) the loss of MnOEP adlayer, allowed the exposure of Au surface, paired with (4) a newly formed MnO_x phase showing the synergistic effect on OER activity. In addition, (5) the enhanced catalytic activity has been reduced after the acid treatment (1:1 solution of HNO_3:H_2SO_4) to remove the MnO_x complexes, but not after the acetone treatment. In summary, we observed the formation of the real active metalloporphyrin-based catalyst, providing a comprehensive picture of the electrocatalytic process and a new impetus for developing the next-generation energy devices.

Poster Presentation : **PHYS.P-227**
Physical Chemistry
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Bimetallic NiPd alloy nanoparticles as electrocatalysts by plused laser reduction method

Chae eun Park, Yeryeong Lee, Yewon Oh, Sieon Jung, Hyeyeon Lee, Yiseul Yu[1], Gyoung Hwa Jeong, Myong Yong Choi*

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

We synthesized NiPd catalysts with high performance of the ethanol oxidation reaction (EOR) by using an unfocused pulsed laser (wavelength 532 nm and power 180 mJ). Also, we tried to measure the electro-conversion efficiency as catalysts with various volume ratio of Ni and Pd: 1:1. 4:1, and 1:4. From a variety of analytical techniques such as scanning electron microscopy (SEM), X-ray diffractometer (XRD), Transmission Electron Microscopy (TEM) and soon, we observed the well-made alloys nanoparticles with ca. 2nm. In addition, our alloy nanoparticles were used as electrocatalysts in field of the ethanol oxidation reaction (EOR) to investigate potential efficiencies. Among NiPd alloys, Ni:Pd (1:1) exhibited higher ethanol oxidation reaction (EOR) activity than commercial Pd/C. In conclusion, we could synthesize the well-defined NiPd alloy nanoparticles via pulsed laser reduction technique. Furthermore, the laser synthetic method is eco-friendly method, and has a potential effect on the surface of nanoparticles as compared with common wet chemical methods.

Poster Presentation : **PHYS.P-228**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

In-situ observation of the Pt-CoO interface in PtCo bimetallic nanoparticle for the CO oxidation

Yejin Song, Jeong Young Park*

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

Bimetallic catalysts exhibit higher catalytic activity than monometallic catalysts due to their bimetallic synergy. In a Pt-3d transition metal (TM, e.g., Ni, Fe, and Co) bimetallic catalytic system, the atomic restructuring occurs at the surface and affects the electronic structure and catalytic activity. The previous research into the surface restructuring of PtCo nanoparticles observed that Co atoms migrated to the nanoparticle surface and CoO island was formed during oxidation. Furthermore, the enhanced catalytic activity of PtCo nanoparticles during the hydrogen oxidation reaction was found to be due to the presence of Pt-CoO interface. The strong metal-support interaction of Pt-3d TM oxide interfacial structure could explain the catalytic improvement in bimetallic catalysts. Therefore, in this study, we synthesized 4 nm PtCo bimetallic nanoparticles with different compositions (Pt:Co = 3:1, 1:1, 1:0) by the polyol method. These nanoparticles were applied to CO oxidation reaction and the result of catalytic performance was shown in the following order: Pt_3Co_1, Pt_1Co_1, and Pt. PtCo bimetallic catalysts were superior to Pt monometallic catalyst, and Pt_3Co_1 was the best among them. *In-situ* analysis, ambient pressure X-ray photoelectron spectroscopy and diffuse reflectance infrared Fourier-transform spectroscopy, were used to prove the relationship between the interface of Pt-CoO and enhanced catalytic performance of PtCo bimetallic nanoparticles. These results of *in-situ* analysis demonstrate that the presence of metal-oxide interfaces contributes greatly to enhancing the catalytic activity.

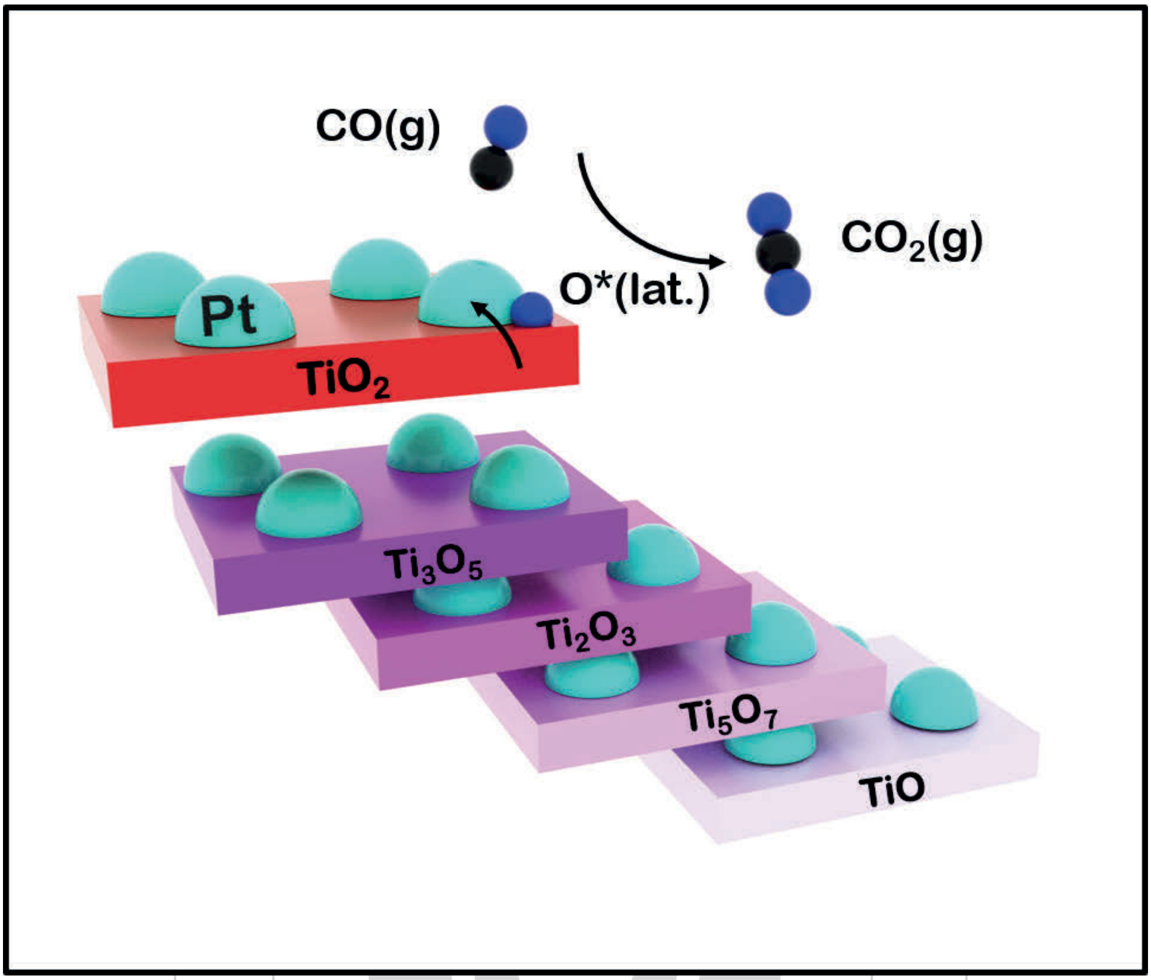
Poster Presentation : **PHYS.P-229**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effect of Support Oxidation State on Catalytic Activity of Pt/TiO_x Catalysts

Gyuho Han, Jeong Young Park[*]

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

The interaction between metal and support is well known to have substantial enhancement on catalytic activity. One of the reasons for this phenomenon is the oxygen-providing property of oxide support, which promotes reaction via the Mars-van Krevelen (MvK) mechanism. Herein, we investigate the effect of support's composition with two-dimensional Pt/TiO_x catalysts using carbon monoxide (CO) oxidation reaction. Titanium oxide films with five different compositions were prepared by an e-beam evaporator, using TiO_2, Ti_3O_5, Ti_2O_3, Ti_5O_7, TiO granules. Then, we directly deposited platinum nanoparticles without any capping layer by arc plasma deposition (APD). With CO oxidation reaction, we checked apparent differences of turnover frequency (TOF) and activation energy between samples. Among five samples, Pt/TiO_2 showed the highest TOF and lowest activation energy. TOF and activation energy of other samples lined up with descending order of oxidation state of titanium. Also, to investigate the interfacial effect between catalyst and support, we deposited Pt on TiO_x films via sol-gel method and compared them with APD deposited samples. By comparing them, we checked the higher catalytic ability of APD samples, which indicates interfacial site enhances catalytic activity. By kinetics study conducted with varying CO pressure, we confirmed that the reaction mainly goes with MvK mechanism. Overall, this research shows that support composed of more oxygen and catalyst with more interfacial sites is better to provide oxygen and promotes the reaction via MvK mechanism.


CO(g)
CO$_2$(g)
O*(lat.)
Pt
TiO$_2$
Ti$_3$O$_5$
Ti$_2$O$_3$
Ti$_5$O$_7$
TiO

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Physical Chemistry
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Nanoscale Friction of Intercalated Water Layers Between Exfoliated MoS2 and Mica

Dooho Lee, Jeong Young Park*

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

In friction force microscopy (FFM), hydrophilicity is an important factor since friction coefficient and adhesion force are dependent on humidity due to capillary condensation between cantilever and sample. In contact mode atomic force microscopy (AFM), water molecules at the surface are unobservable since they are displaced by the cantilever. During exfoliation of 2D materials such as graphene or molybdenum disulfide (MoS2), those water layers are intercalated between 2D material and hydrophilic substrate, and thus can be visualized by AFM imaging. Intercalated water layers between hydrophobic graphene and mica are known to increase friction by providing additional excitation channel, and this effect is screened with increasing graphene layers above water layers. Water layers intercalated between mica and hydrophilic MoS2 grown by chemical vapor deposition (CVD) are also known to increase friction, but tribological properties including layer dependence have not been studied. Furthermore, difference in adhesion and crystalline qualities between exfoliated MoS2 and CVD-grown MoS2 can lead to difference in frictional properties. In this research, we quantitatively examined the tribological effect of water layers intercalated between exfoliated MoS2 and mica. Despite different structure and physical properties including hydrophilicity, intercalated water layers under MoS2 showed similar frictional effect with the case of graphene. This result shows that atomic layers covering water do not play important role for the friction change and makes it possible to expect the general trend of nanotribological properties of water intercalated 2D materials.

Poster Presentation : **PHYS.P-231**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effects of Water Vapor on Oxidation Process of Cu(111) Surface and Sublayer

Youngjae Kim, Jeong Young Park*

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

Copper-based materials were studied for catalytic reactions with different oxidation states. A transition of the oxidation states is involved in some reaction mechanisms. Here, we report the observations of oxidation processes on a Cu(111) single crystal by using near-ambient pressure scanning tunneling microscopy (NAP-STM) and X-ray photoelectron spectroscopy (NAP-XPS) to understand real reaction conditions. Until 0.1 mbar of water vapor conditions, there were no significant changes on Cu(111) surface morphologies. The Cu(111) surface started to be oxidized at 0.01 mbar of a pure O_2 environment. Time-lapse NAP-STM and NAP-XPS results displayed that the dry oxidation was initiated at step edges as a form of unstable adsorbed oxygen atoms, $O_{(ad)}$, and progressed to terrace by Cu_2O phase. After that, independent oxidation on the Cu(111) terrace were observed. For H_2O/O_2 mixed gas conditions, the humid oxidation on the Cu(111) surface occurred at 0.02 mbar. Time-lapse NAP-STM images demonstrated that the oxidation also proceeded from the step edges to the terrace, but there were no independent oxidations. Time-lapse NAP-XPS results showed that the appearances of chemical species were similar to the dry oxidation. Hydroxides and adsorbed water molecules were observed after the surface was saturated as Cu_2O phase. We found that the depth of Cu_2O was dramatically different in the dry and humid oxidation by analyzing the relative intensity and peak area of XP spectra. The Cu_2O depth of the dry oxidation was greater than that of the humid oxidation. The step edge coverage of the Cu_2O layer was different, which activated the supplement of oxygen atoms to the Cu(111) sublayer.

Poster Presentation : **PHYS.P-232**
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Atomic-Scale Gliding On Hydrophilic Surfaces at High Humidity Observed by Friction Force Microscopy

Tae Won Go, Jeong Young Park*

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

The effect of adsorbed water layers on the frictional properties of hydrophilic surfaces with respect to graphene in various relative humidities (RH) was investigated by friction force microscopy (FFM). In moderate RH (53.1 %), graphene and silica showed clear contrast in topography, and friction on silica was higher than that on graphene. The abundance of water on silica in high RH (98.2 %) blurred the topographical contrast between graphene and silica, but they could still be distinguished from the friction image. The friction value on silica as a function of humidity relative to graphene showed a peak in an intermediate RH (~63.4 %) and then decreased as the humidity increased. This humidity dependence of friction was also confirmed in the case of mica and graphene. In RH higher than 98.2 %, friction on silica was lower than that on graphene, which indicated the gliding of AFM tip on the adsorbed water layers on silica. Additionally, the enhancement of friction on the water-intercalated graphene as a result of more efficient phonon-mediated energy dissipation was observed. These results suggest that adsorbed water layers at probe/hydrophilic surface in high RH can overcome the capillary and viscosity effects and thus lead to the occurrence of atomic-scale gliding. We hope that our findings may provide useful insights for applications of hydrophilic surfaces in ambient conditions.

Poster Presentation : **PHYS.P-233**
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Formation of catalytically active Au-CuO_x heterostructure by oxygen-induced atomic restructuring

TaekSeung Kim, Jeong Young Park[1,*]

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

In classical chemistry, gold (Au) was regarded as an inactive heterogeneous catalyst due to high ionization potential and low interaction with other elements for a long time. However, the conventional scientific perception was broken by the introduction of Au nanochemistry for size- and support-dependency in heterogeneous catalysis reported by Prof. Haruta and Hutchings. For 3d-metal oxide supported Au nanocatalyst, the changed electronic structure at the interface between Au and 3d-metal support contributes to the highly active catalytic thermodynamics. Diverse studies for Au nanochemistry are actively progressed, but understanding the catalytic mechanism remains an important issue. Here, we report a strategy to understand the dynamics in Au nanochemistry for oxidation and CO conversion using a bimetallic synergy in Au–Cu nanocrystal. Atomic restructuring of Au–Cu nanocrystal in oxidation environment is comprehensively investigated using combined operando spectroscopic (near-ambient-pressure X-ray photoelectron spectroscopy; NAP-XPS and diffuse reflectance infrared Fourier-transform spectroscopy; DRIFT) and in situ microscopic (environmental transmission electron microscopy; ETEM) analysis, resulting in the formation of CuO_x/Au–Cu heterostructure. Then, the formation of heterostructure and its catalysis for CO oxidation were rationalized by density-function theory (DFT) calculation. Our results indicate that the heterostructure with a metal-oxide interface is closely connected to enhancing the catalytic activity regarding the electronic metal-support interaction (EMSI) effect.

Poster Presentation : **PHYS.P-234**

Physical Chemistry

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Detection of thiram via Cl^- ion adsorbed light-induced growth of AgNPs-cellophane substrate

Rashida Akter, Kwanghyeon Jo, Deun Chan Lee, Trinh Ba Thong, Joan Monteroso, Ilsun Yoon[*]

Department of Chemistry, Chungnam National University, Korea

We developed a new plasmonic chloride (Cl^-) ion treated silver nanoparticles (AgNPs) deposited cellophane paper (CP) substrate by growing the AgNPs through light induced reduction of pre-deposited Ag ions on CP. The AgNPs/CP substrate was characterized using UV-vis spectroscopy, scanning electron microscopy, and energy dispersive X-ray microscopy. The substrate showed a high surface coverage of AgNPs with hierarchical morphology. The CP/AgNPs substrate exhibited strongly enhanced SERS activities of benzenethiol (BT) with the enhancement factor (EF) of 1.2×10^7 with a relative standard deviation (RSD) of 6.7%. The AgNPs/CP substrate was successfully applied for ultrasensitive SERS detection of a model pesticide, thiram in deionized (DI) water. The results show that the light induced AgNP deposited CP-based SERS substrate could selectively and reproducibly detect thiram with a LOD of 0.24 nM (0.057 ppb) and a RSD of 5.2% in DI water.

Poster Presentation : **PHYS.P-235**
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Computational study on the photophysical properties of thermally activated delayed fluorescent molecules due to regiochemical configuration

Taehwan Lee, Young Hoon Lee, Min Hyung Lee*, Jaehoon Jung*

Department of Chemistry, University of Ulsan, Korea

Efficient triplet-to-singlet upconversion by reverse intersystem crossing (RISC) plays a crucial role in realizing high performance the thermally activated delayed fluorescence(TADF)-OLEDs. Hence, it is typically desirable for TADF emitters to have a small energy splitting (ΔE_{ST}) between the excited singlet (S_1) and triplet (T_1) states for fast RISC. However, the strong spin orbit-coupling (SOC) between charge transfer ($^1CT(S_1)$) and local excited ($^3LE(T_n)$) states governed by El-Sayed's rule has been recently reported to be of importance in achieving a fast reverse intersystem crossing (k_{risc}) process. We experimentally reported that the regioisomers of D-A type TADF-molecules have different photophysical properties. Herein, we study how the *ortho* and *para* regiochemical configurations between donor and acceptor moieties influence their photophysical properties using density functional theory (DFT) calculations [1,2]. We elucidated that the *ortho* configuration can result in small ΔE_{ST}, and furthermore the T_2-mediated RISC process can play a role as a dominant channel of TADF process due to high SOC matrix element. The range separated hybrid functional ω*B97X-D with ω-tuning method in solution (toluene) medium was utilized to evaluate the photophysical properties. We expect that this work can provide a way to understand the regiochemical dependence of TADF process and to rationally design the TADF molecules.

[1] Y. H. Lee, S. Park, J. Oh, J. W. Shin, J. Jung, S. Yoo, and M. H. Lee, ACS Appl. Mater. Interfaces 2017, 9, 24035−24042.
[2] Y. H. Lee, Y.-S. Shin, T. Lee, J. Jung, J.-H. Lee, and M. H. Lee, Chem. Eng. J. 2021, 423, 130224.

Poster Presentation : **PHYS.P-236**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Excited state reaction dynamics of dye-aggregates on TiO_2 particle probed by ultrafast time-resolved fluorescence

Yun Jeong Na, HyunJae Lee, Ho-Jin Son*, Chul Hoon Kim*

Department of Advanced Materials Chemistry, Korea University, Korea

Understanding charge injection dynamics of a photosensitizing organic dye anchored on TiO_2 nanoparticles is essential to improve the performance of dye-based solar energy conversion systems. In this study, we have fully investigated photo-physical properties of a coumarin dye, 7-hydroxycoumarin-3-carboxylic acid, in both aqueous solution and thin solid film by time-resolved fluorescence spectroscopy. In aqueous solution, it was confirmed that there is the chemical equilibrium between dye monomers and their aggregates, and the portion of the dye aggregates is highly influenced by pH. The blue-shifted absorption spectrum of the aggregate was gradually decreased by adding NaOH solution, and it was completely converted to the monomer (anion form) when 1 eq. of NaOH was employed. In film, steady-state and time-resolved fluorescence spectroscopy measurements were conducted. The isolated monomer film, which is prepared on the TiO_2 surface with excess Chenodeoxycholic acid (CDCA), only showed ultrafast charge-injection with about 100 fs time-scale with minor spectral shift. The aggregated one, however, exhibited additional population relaxation to lower-lying excited state to show characteristic dual emission. This might be competing with the charge injection into the TiO_2 conduction band. We took a care to determine the relaxation time by direct measurement of femtosecond time-resolved spectra, and tried to elucidate how the relaxation process affects the dye-sensitized solar cell (DSSC) efficiency.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **PHYS.P-237**

Physical Chemistry

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[Withdrawal] Active Transport Dynamics in Neuron Cells: Order and Disorder

Donghee Kim, **Ji-Hyun Kim**[1], **Jaeyoung Sung**[1,*], **Kang Taek Lee**[2,*]

Chemistry, Chung-Ang University, Korea
[1]*Department of Chemistry, Chung-Ang University, Korea*
[2]*Department of Chemistry, Gwangju Institute of Science and Technology, Korea*

- Withdrawal -

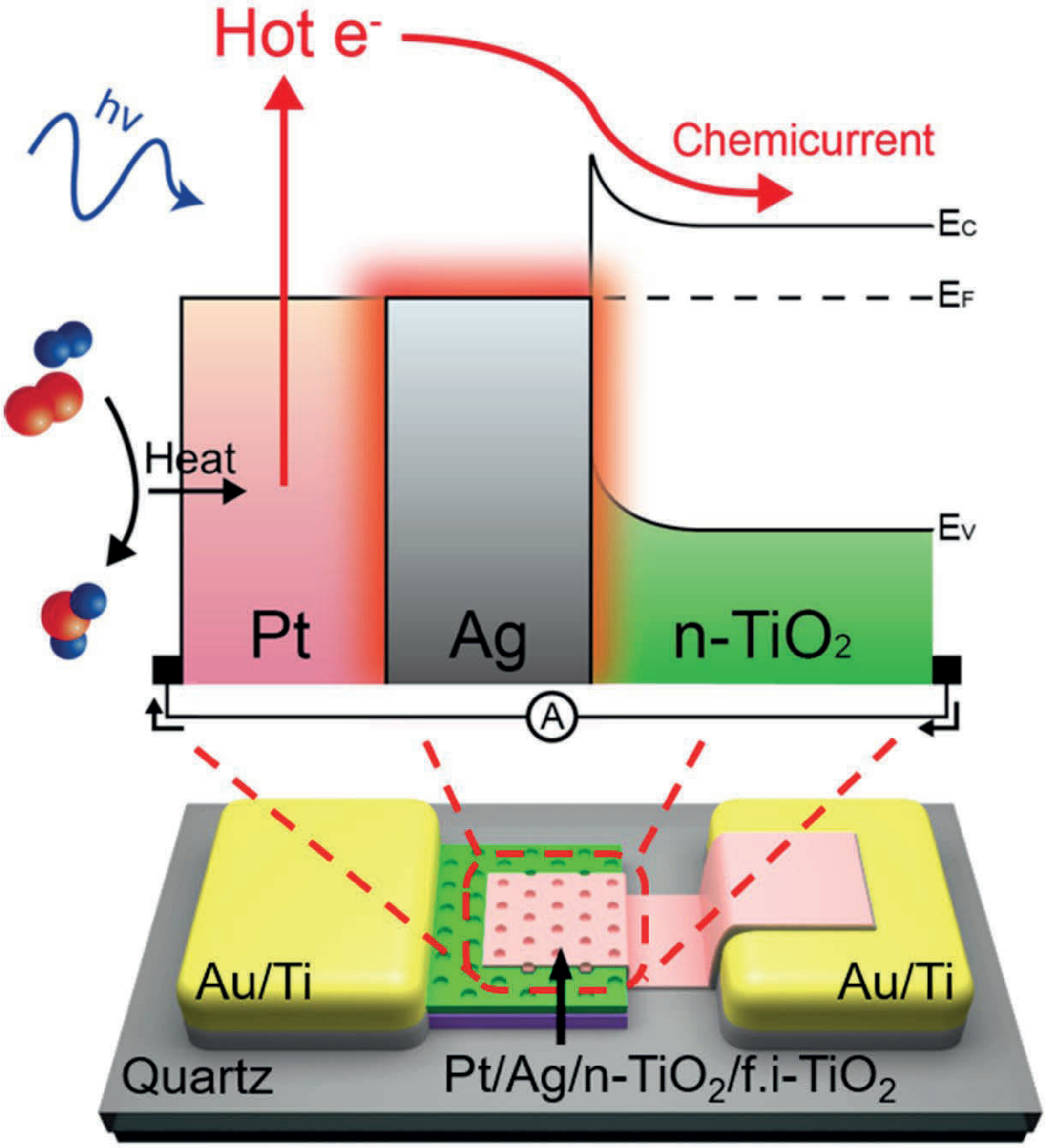
Poster Presentation : **PHYS.P-238**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Pt/Ag/TiO_2 Plasmonic Nanodiodes for Extraction of Surface Plasmon-driven Chemicurrent

Mincheol Kang, Jeong Young Park*

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

In order to overcome an energy crisis, solar energy conversion in the field of photocatalysis is actively researched, and photocatalyst design incorporating surface plasmon is drawing significant attention as a highly competitive catalyst system. Important factors of surface plasmon are size, shape, and material of plasmonic metal nanostructures, which affect plasmonic excitation, absorbance, and hot electron collection. In this study, we fabricated the ordered structure of metal-semiconductor plasmonic nanodiodes with size control using nanosphere lithography and reactive ion etching. Plasmonic nanodiodes composed of Pt/Ag/TiO_2 were used to detect exothermic surface reaction-induced hot electrons (chemicurrent) enhanced by the plasmonic effect under the hydrogen oxidation. In this system, the surface temperature was measured using the thermovision to distinguish contributions of the plasmonic effect and the photothermal heating effect. When the light of the particular wavelength region (400~500 nm) is incident on the diodes, both chemicurrent and catalytic activity of hydrogen oxidation were amplified by the plasmonic effect of antenna Ag. In addition, the plasmonic effect is visually exhibited using the finite difference time domain simulations. The novel scheme of antenna-reactor using plasmonic nanodiodes may offer a strategy for advanced hot-electron-based catalytic and photovoltaic devices.


hν
Hot e⁻
Chemicurrent
Ec
EF
Ev
Heat
Pt
Ag
n-TiO₂
A
Au/Ti
Au/Ti
Quartz
Pt/Ag/n-TiO₂/f.i-TiO₂

Poster Presentation : **PHYS.P-239**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Impact of Hot Hole Transport on Photocatalytic Activity in Au Nanoprisms/p-GaN under Water Splitting Reaction

Kyoungjae Song, Jeong Young Park[1,*]

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

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

Under the irradiation of light, excited carriers with high kinetic energy (1-3 eV) can be generated in plasmonic metals. The carriers consist of hot electrons and hot holes. The hot holes have a considerable potential due to their more energetic kinetics relative to hot electrons. To utilize hot holes by localized surface plasmon resonance, a plasmonic metal/ p-type semiconductor Schottky platform was proposed. Utilizing Au nanoparticle/ p-GaN photocathode, hot holes can be detected and photocatalytic reaction by hot holes can also be measured.To investigate the correlation between photocatalytic activity and hot holes by surface plasmon, we fabricated size-controlled Au nanoprisms/ p-GaN photocathode using an e-beam evaporator. The electrical properties of the platform were measured by the conductive atomic force microscopy and Kelvin probe force microscopy. The triangle-shaped Au has a thickness of 10 nm and a length of 90 nm, 140 nm, and 220 nm. The small-sized Au nanoprism exhibited a high external quantum efficiency by a factor of 2 compared to that of the large one. We found that the amount of hydrogen and oxygen gas evolution increased as the size of Au nanoprism decreased from 220 nm to 90 nm. The results indicate the enhanced hot hole flux by amplification of localized surface plasmon resonance leads to the promotion of hydrogen and oxygen gas evolution reaction.

Poster Presentation : **PHYS.P-240**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Facet-dependent strong metal-support interaction of Pt nanoparticle on morphology controlled Cu_2O for CO oxidation

Seunghwa Hong, Jeong Young Park[*]

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

Supported metal catalysts, which have form of noble metal nanoparticles supported on metal oxide, are widely used as heterogeneous catalyst in industrial chemical production. It is well-known that the interaction between metal nanoparticle and metal oxide, so called as strong metal-support interaction (SMSI), takes central part in engineering catalytic behavior of the catalyst due to the synergistic effects on catalytic activity at the metal-oxide interface. Thus, fundamental understanding of SMSI in the realistic reaction condition is important to modify the catalytic property via fine tuning of the SMSI. However, direct investigation of the SMSI is challenging due to the structural complexity of the heterogeneous catalysts. Facet-controlled metal oxide crystals, such as TiO_2, Co_3O_4, and Cu_2O, are a good candidate to study the SMSI at the metal-oxide interface since their surface possesses well-defined structure.Herein, we investigated facet-dependent SMSI at Pt nanoparticles supported on cubic and octahedral Cu_2O using surface-sensitive *operando* techniques. Catalytic measurement revealed that the interface of Pt/cubic-Cu_2O gives larger enhancement on the catalytic activity than that of Pt/octahedral-Cu_2O. The results of *in-situ* ambient pressure X-ray photoelectron spectroscopy and diffuse reflectance FT-IR spectroscopy indicate that the surface changes during the reaction depends on the facet of the support, leading to different catalytic performance. These results demonstrate facet-dependent SMSI effects at the Pt-Cu_2O interface, further providing efficient platform to engineer SMSI by controlling the facet of the support.

Poster Presentation : **PHYS.P-241**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Operando investigation of strong metal-support interaction at the interface of Pt-Co_3O_4 during CO oxidation

Daeho Kim, Jeong Young Park*

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

Noble metal nanoparticles (NPs) on transition metal oxide supports (e.g., Co_3O_4, NiO, TiO_2, CeO_2, and Fe_2O_3) have been widely used as a heterogeneous catalyst for reinforcing catalytic activity and adjusting the reaction mechanism of various catalytic reactions such as CO oxidation, CO_2 hydrogenation, and Fischer-Tropsch process. The unique interaction at the interface of the metal NP and oxide, which known as the strong metal-support interaction (SMSI), gives synergistic enhancement to the catalytic performance. Therefore, a fundamental understanding of SMSI during catalytic reaction using operando surface characterization is demanded to develop high-performance heterogeneous catalysts.Herein, we show the direct evidence of SMSI state at the interface of Pt NP and Co_3O_4 utilizing operando surface analysis. The Pt-Co_3O_4 interfaces were constructed as three-dimensional catalyst system using Pt NPs embedded on the mesoporous Co_3O_4. The two-dimensional model system is also prepared via a Langmuir-Blodgett trough to investigate the origin of SMSI. The *ex-situ* transmission electron microscopy reveals that the surface of Pt NPs was encapsulated by Co_3O_4 overlayer after CO oxidation. The *operando* surface analysis and computational calculation using ambient pressure X-ray photoelectron spectroscopy, diffuse reflectance infrared Fourier-transform spectroscopy, and density functional theory indicate that the interface of Pt NP and Co_3O_4 thin overlayer is key state of the SMSI enhancing the catalytic activity.

Poster Presentation : **PHYS.P-242**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Highly-sensitive quantification of metal chelating activity

Sangmin Ji, Hye Ran Koh[*]

Department of Chemistry, Chung-Ang University, Korea

Metal ions play an important role in various physiological processes. Some ions act as a cofactor to control the catalytic activity of many enzymes and contribute to various genetic processes by stabilizing the secondary structure of DNA and RNA. Moreover, the abnormal amount of many heavy metal ions are related with diseases such as Parkinson’s disease, Alzheimer’s disease and cancer and chelating reagents to inactivate the metal ions are often treated as a drug for those diseases. To monitor the efficacy of the chelating therapy, the quantification of the metal-chelating activity is required. In this study, we achieved to detect the low concentration of divalent metal ions with high precision by observing the conformational change of a hairpin DNA probe using single-molecule fluorescence resonance energy transfer technique, which depends on the concentration of the divalent ions. We managed to calculate the chelating efficiency and obtain the binding affinity of various chelating reagents including ethylenediaminetetraacetic acid (EDTA), ethylene glycol-bis(β-aminoethyl ether)-N,N,N’,N’-tetraacetic acid (EGTA), 1,2-bis(2-aminophenoxy)ethane-N,N,N’,N’-tetraacetic acid(BAPTA) by measuring the remaining divalent ions after the treatment of each chelating reagents. We found that the calcium-specific chelating reagents such as EGTA and BAPTA showed the higher binding affinity to calcium ions than magnesium ions while the EDTA showed the relatively similar metal specificity. This assay takes less than 5 mins, which could work as a useful platform to screen the efficacy of the metal-chelating drugs, suggesting the guideline for their development.

Poster Presentation : **PHYS.P-243**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Ultrasensitive detection of single base substitution mutation by combining CRISPR-Cas system and single-molecule fluorescence detection

Seohyun Kim, Hye Ran Koh*

Department of Chemistry, Chung-Ang University, Korea

Single base substitutions or point mutations , where one base pair is swapped by a different base pair, represent up to 85% of the oncogenic mutations in cancers. In this respect, ultrasensitive detection of single base substitutions is highly needed to diagnose the mutation-associated genetic diseases even at its early stage. Here, we reported the ultrasensitive detection method of a single base substitution mutation, which combines the advantages of DNA targeting specificity of CRISPR-Cas system and the single-molecule detection sensitivity of total internal reflection fluorescence microscopy. CRISPR-Cas system, the immune system of the bacteria and archaea, binds and cleaves the target DNA that has both an appropriate protospacer adjacent motif (PAM) sequence and complementarity to guide RNA (gRNA) sequence. We employed the deactivated Cas9 (dCas9) protein which loses the endonuclease activity but still possesses the sequence-specific DNA binding activity and designed gRNA to locate the point mutation of target DNA in PAM region for discrimination of mutation from wild type. We applied our assay to detect the point mutation of the EGFR c.2573T>G causing lung cancer and observed much more binding of dCas9-gRNA complexes to the target DNA with the point mutation than wild-type DNA. With the varied ratio of mutation to wild type, we showed that the quantitative measurement of the point mutation was possible over all the range of the ratio from 0 to 100 % and successfully discriminated the minor allele even down to 0.5 %, approximately 100 fM in concentration. We also detected the other point mutations in KRAS gene that are frequently found in lung cancer, which suggests the universality of our assay in detecting point mutations.

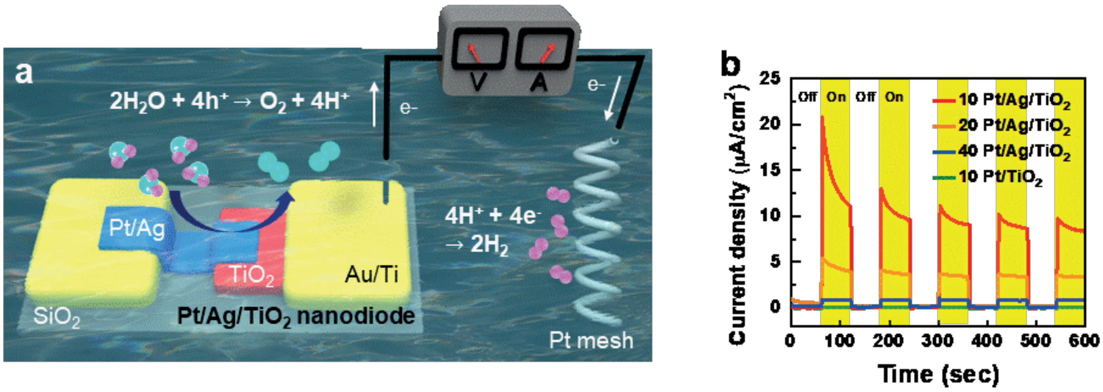
Poster Presentation : **PHYS.P-244**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Role of plasmonic hot carriers in photoelectrochemical water splitting using antenna-reactor Pt/Ag/TiO_2 Schottky nanodiodes

Heeyoung Kim, Jeong Young Park[*]

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

Plasmon-assisted photoelectrochemical (PEC) water splitting has been actively studied in developing the plasmonic metal-semiconductor (SC) Schottky heterostructures to improve the light absorption capacity and the catalytic activity of the photoelectrodes. Moreover, it has been recently reported that plasmonic metal(antenna)-cocatalyst(reactor) nanostructures can play a critical role by which the plasmonic metal enhances harvesting the incident photon and the cocatalyst boosts the catalytic reaction. Here, we fabricated antenna-reactor type Pt/Ag/TiO_2 metal-SC Schottky nanodiodes to detect the hot carriers and elucidated the effect of plasmonic hot carriers on PEC water splitting. As shown in Figure a, when the visible light illuminates upon the Pt/Ag/TiO_2 nanodiode photoanode, the plasmonic hot carriers are generated in plasmonic Ag, and the energetic hot electrons overcome the Schottky barrier, and hot holes go to Pt surface after charge separation. Hot holes participate in oxygen (O_2) evolution reactions on the Pt/Ag/TiO_2 photoanode surface, while hot electrons are transferred through the circuit and utilized for hydrogen (H_2) evolution on the cathode. To prove the effect of plasmonic carriers on overall PEC water splitting, 3 different Pt/Ag/TiO_2 photoanodes were prepared by controlling the thickness of the Pt film as 10, 20, 40 nm deposited on plasmonic Ag. As shown in Figure b, the chronoamperometry measurements showed that as the thickness of the Pt was decreased, the photocurrent density was increased. The photocurrent of 10 Pt/Ag/TiO_2 was 8.4 A/cm^2 which is 2.5 and 10.5 times higher than that of 20 Pt/Ag/TiO_2 and 40 Pt/Ag/TiO_2, respectively. We also confirmed that the efficient extraction of the plasmonic hot holes and fast charge transfer in 10 Pt/Ag/TiO_2 photoanode from the results of the incident to photon efficiency (IPCE) and electrochemical impedance spectroscopy (EIS). Lastly, we measured the actual amount of evolved O_2 (5.82 mol) and H_2 (2.91 mol) gas during 60 minutes at 1.5 V vs RHE and the faradaic efficiency of all Pt/Ag/TiO_2 for O_2 and H_2 evolution reaction was over 95%, implying Pt/Ag/TiO_2 photoanode system successfully utilizes plasmonic hot carriers for PEC water splitting. In conclusion, this study demonstrated that the strong electric field confinement of plasmonic Ag and the generated plasmonic hot carriers play a dominant role in enhancing the photocatalytic activity in water splitting.



Poster Presentation : **PHYS.P-245**

Physical Chemistry

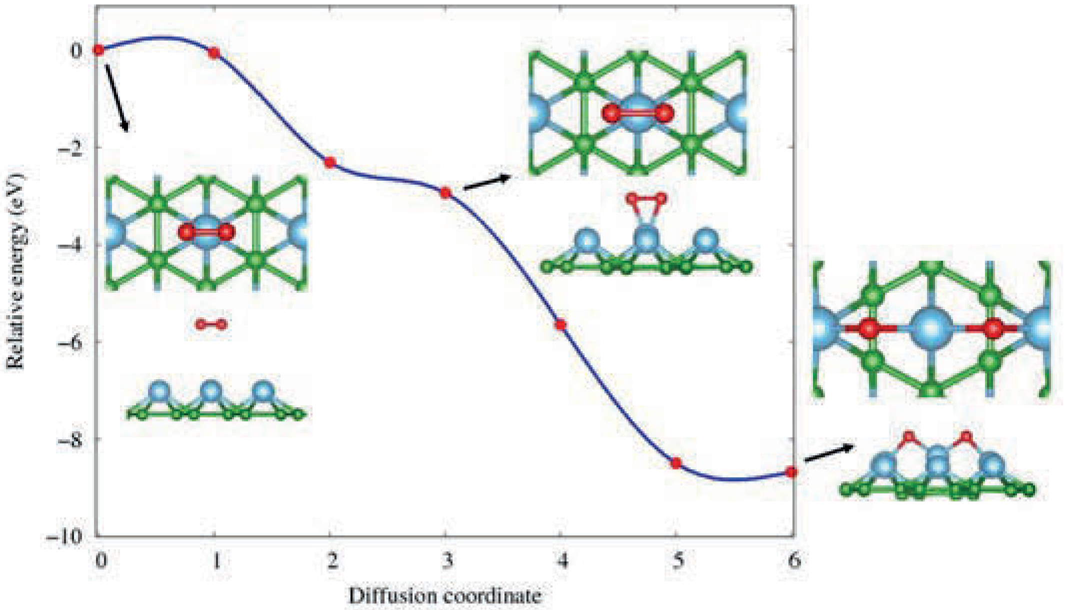
Exhibition Hall 1 THU 11:00~12:30

Adsorption and reaction mechanism of O_2, CO_2 and NO_2 over TiB_2 monolayer

Mahbubul Alam Shoaib, Jaehoon Jung[*]

Department of Chemistry, University of Ulsan, Korea

There have been many studies on TiB_2, and it was revealed to possess a high chemical stability and many fascinating properties, such as high melting point, low resistance, extreme hardness, and good thermal conductivity. A perfect monolayer of TiB_2 is composed of titanium atoms adsorbed on one side of hexagonal boron monolayer where Ti atoms are fixed due to the strong covalent bonding with B atoms. TiB_2 has a possibility to be more reactive due to the metallic Ti atoms compared to other 2D materials, such as graphene or h-BN. A self-consistent periodic density functional theory (DFT) study is herein performed to get insight into the adsorption processes of O_2, CO_2, and NO_2 on TiB_2, and into the dissociation mechanism of O_2 molecule over the TiB_2 monolayer. It is observed that a barrierless O_2 dissociation occurs due to the strong interaction between the TiB_2 surface and the O_2 molecules. It was also found that the minimum energy path (MEP) for the chemisorption process of CO_2 and NO_2 relies on the adsorption sites. Our computational results indicate that more detailed mechanistic study would be required for elucidating a potential of TiB_2 monolayer as chemical sensor or heterogeneous catalyst.



Relative energy (eV)
0
−2
−4
−6
−8
−10
0
1
2
3
4
5
6
Diffusion coordinate

Poster Presentation : **PHYS.P-246**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Molecular Dynamics Simulation Studies for the Membrane Structure of Glycerolipid and Chlorosulfolipid Mixtures

Janghee Hong, Rakwoo Chang[1,*]

University of Seoul, Korea

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

Chlorosulfolipids (CSLs) are major compounds of flagellar membranes in Ochromonas Danica. They are toxic and are known to be related to Diarrhetic shellfish poisoning. CSLs have various structural isomers, with a charged sulfate group in the middle of the hydrophobic chain. In this study, we used Danicalipin A as a CSL and dippalmitoyl-glyceryl-trimethylhomoserine (DPTS) as a glycerolipid and performed coarse-grained (CG) simulation to gain difference in mixed system with membrane, which is a rare class of glycerolipid that is found in Ochromonas Danica. After few hundred nanoseconds of the CG simulation, we observed that membrane did not self-assemble as CSLs' concentration increased.

Poster Presentation : **PHYS.P-247**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Concentration Effects of Polyhexamethylene Guanidine (PHMG) on Lung Surfactant Membranes: Molecular Dynamics Simulation Studies

Jiyeon Hyun, Rakwoo Chang[1,*]

University of Seoul, Korea

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

Polyhexamethylene guanidine (PHMG) is a guanidine-based chemical that is used as humidifier disinfectants, wet tissues, and non-woven fabrics. It is less toxic to the skin and has sterilization power and dissolves well in water. However, it has been found that if the substance is inhaled and accumulates in the lungs, over time the substance can become toxic in the lung tissue and cause pulmonary fibrosis. In this study, we have performed Molecular Dynamics (MD) simulation to examine the changes in the lung surfactant membrane according to the concentration of PHMG by modeling a monolayer which is composed of dipalmitoylphosphatidylcholine (DPPC), a major component of lung surfactant. The MD simulations were performed with different concentrations by increasing the number of PHMG, mimicking aerosols. We have observed that the water droplets entered the water phase within first 5 ns. However, PHMG did not completely permeate the water phase and was accumulated in the membrane. In addition, as the concentration increased, the membrane was severely deformed, and it was confirmed that the membrane was condensed. Then, we calculated structural and translational functions.

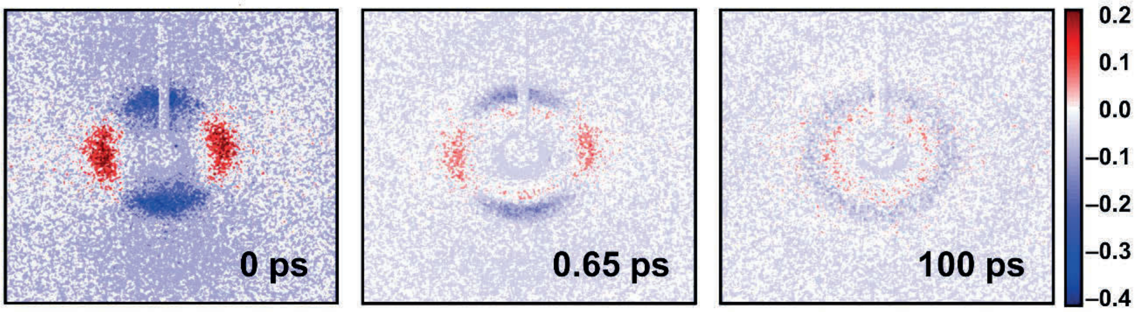
Poster Presentation : **PHYS.P-248**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Ultrafast Dynamics of Optical Kerr Effect in Liquid Acetonitrile Probed by Time-Resolved X-ray Liquidography

Seungjoo Choi, Hyotcherl Ihee[1,*], Jeongho Kim[*]

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

Optical Kerr effect (OKE) is one of the well-studied fields in physics or physical chemistry, and this phenomenon causes change in the refractive index of the material. However, since most of the OKE studies have used spectroscopic techniques to date, structural dynamics have not been directly observed. In view of this, we studied molecular dynamics of OKE in liquid acetonitrile by using femtosecond time-resolved x-ray Liquidography (fs-TRXL). In this experiment, two samples were measured: neat acetonitrile and dye solution in acetonitrile, and the differences in each dynamics were compared. The structural changes in molecules photo-aligned by strong electric field (optical laser pulse) could be described by three distinct motions: libration, orientational diffusion, and interaction-induced motion, these motions could be explained only by the data obtained from fs-TRXL signal, not by theoretical modeling. To back this up, we also compared the scattering signal with molecular dynamic simulation. As a result, the simulated scattering signals from the MD simulation reproduces OKE signals from the measured time-resolved scattering signal well. This experiment is also expected to contribute greatly to future research on fs-TRXL.



Poster Presentation : **PHYS.P-249**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Role of the film thickness on the structural and electronic properties of ultrathin rutile TiO_2 film supported by a metal substrate

Rizky Hadiputra, Jaehoon Jung[*]

Department of Chemistry, University of Ulsan, Korea

Titanium dioxide (TiO_2) has received a great attention due to its importance in a wide variety of applications, such as photocatalysis and solar energy conversion. In particular, the film thickness, as a controllable factor, can play an important role in determining various chemical and physical properties of oxide films, such as catalytic and dielectric properties. In this study, we perform dispersion-corrected density functional theory calculations employing PBE-D3 and projected augmented wave (PAW) method implemented in VASP software package to investigate the geometric and electronic properties of ultrathin rutile titanium dioxide film supported by a metal substrate, $TiO_2(110)/M(100)$ (M = body-centered cubic transition metal). We constructed the model system of n-ML rutile $TiO_2(110)$ film (n = 1-3) supported by (2x1)-M(100) substrate in order to find a proper substrate for realizing a stable rutile TiO_2 film, in which the lattice mismatches between TiO_2 and metal substrate for long and short axes are 1.52~13.44% and 2.31~10.30%, respectively. We found that Mo and W are capable to from a stable TiO_2 film with a strong interfacial interaction. Our results provide a deep insight into the effect of the film thickness on the geometric and electronic properties of rutile TiO_2 film grown on metal substrate.

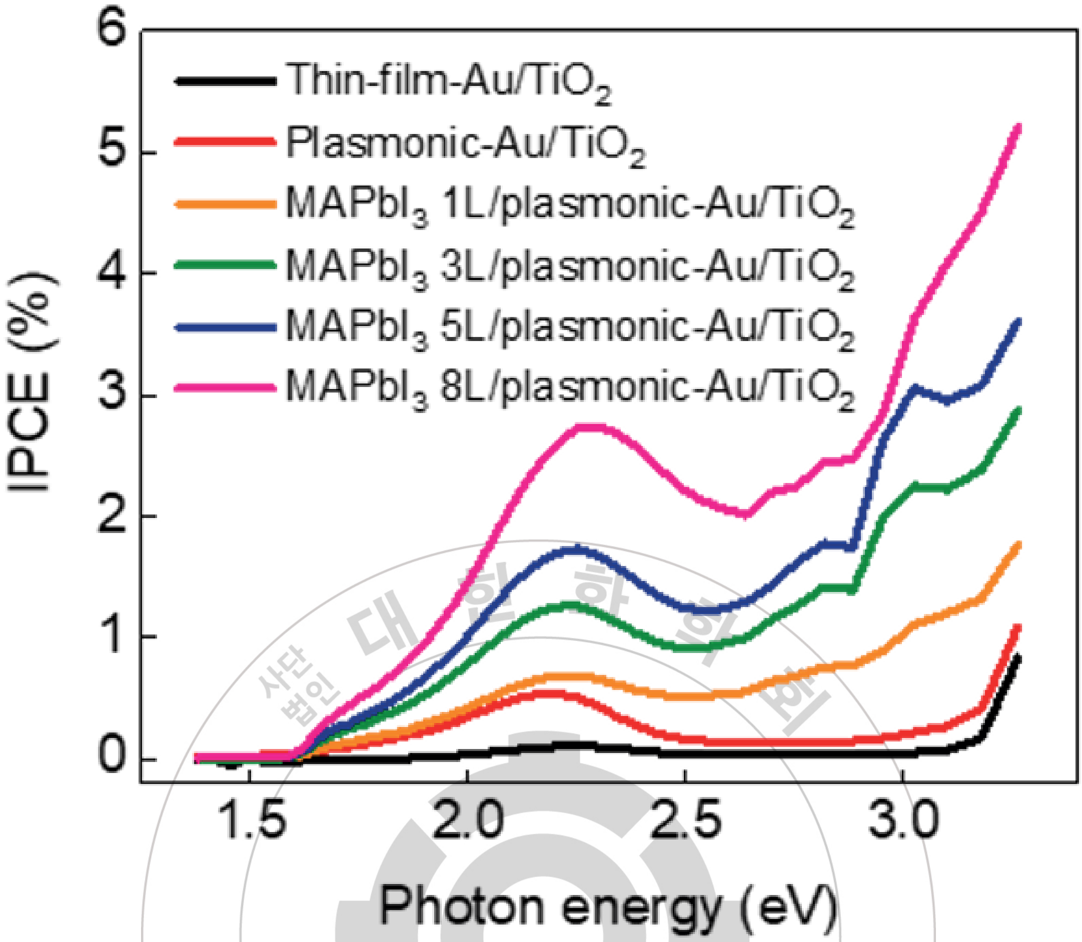
Poster Presentation : **PHYS.P-250**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Prolonged Lifetime and Enhanced Flow of Hot Electrons on a Perovskite Combined Plasmonic Nanodiode

Yujin Park, Hyotcherl Ihee*, Jeong Young Park*

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

Collecting plasmon-induced hot electrons on metal nanoparticles has been extensively investigated in the field of photovoltaics and photocatalysts due to their outstanding photoelectrical properties. However, the ultrafast thermalization of hot electrons prevents their applications from reaching practical levels. In this regard, hybrid perovskite materials have been reported as a strong candidate for hot-electron applications due to their slow hot-carrier relaxation dynamics.In this study, we demonstrate perovskite-combined plasmonic metal (Au and Ag) nanodiode to show the enhanced flow of hot electrons, which is associated with the prolonged hot-electron lifetime. The enhanced hot electron flow and the origin of each hot-electron flux were analyzed by measuring photocurrents and incident photon-to-electron efficiency (IPCE), respectively. Furthermore, the ultrafast pump-probe spectroscopy revealed the prolonged hot-electron lifetime on perovskite modified plasmonic metal structures. By comparing the MAPbI3 coupled with plasmonic Au and that with plasmonic Ag, we found that the latter one is much more beneficial to enhance hot-electron flux due to the intense optical response of plasmonic Ag and facilitated hot-electron transfer. We suggest our results provide insight into the correlation between hot-electron lifetime and flow, which can be useful information to design efficient hot-electron-based photovoltaics.



6
5
4
3
2
1
0
IPCE (%)
1.5
2.0
2.5
3.0
Photon energy (eV)
Thin-film-Au/TiO_2
Plasmonic-Au/TiO_2
$MAPbI_3$ 1L/plasmonic-Au/TiO_2
$MAPbI_3$ 3L/plasmonic-Au/TiO_2
$MAPbI_3$ 5L/plasmonic-Au/TiO_2
$MAPbI_3$ 8L/plasmonic-Au/TiO_2

Poster Presentation : **PHYS.P-251**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Photoluminescence blinking and photostability of perovskite quantum dots in a single nanoparticle level

Weon-Sik Chae

Daegu Center, Korea Basic Science Institute, Korea

Recently, perovskite nanomaterials have attracted increasing attentions because of its tunable band-gap in visible region, absorption coefficient, and high emission quantum yield. A facile synthetic routes and scalable production enabled important application areas such as solar energy conversion and light emitting display. However, the soft characteristics (ion mobility, phase separation, and decomposition) of the perovskite phase restricted the potential applications in the aspect of durability. Hence, we have studied photophysical properties of the perovskite quantum dots (green and red colors) through photoluminescence (PL) blinking, time-trace PL lifetime modulation, and time-elapsed photostability experiments. Interestingly, the results indicate a single perovskite quantum dots suffer multiple recombination routes even in a signle particle. We would like to discuss further about cross correlation between photoluminescene blinking and photostability of perovskite quantum dots.

Poster Presentation : **PHYS.P-252**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Characterization of Gas Separation Amorphous Polymers Using Molecular Dynamics: Impact of Spacer on Gas Separation Performance

Sanggil Park, Hyungjun Kim*

Department of Chemistry, Incheon National University, Korea

The emission of carbon dioxide is causing serious problems such as global warming, sea level rise, and ocean acidity increase. In order to solve this problem, it is highly desirable to remove carbon dioxide from atmosphere. Amongst various approaches, an amorphous polymer-based gas separation membrane is attracting attention owing to alternatives it has advantages in that energy consumption is low and easy to increase in size. Gas separation membrane polymers are required to have various characteristics, among which permeability and selectivity are the most important characteristics that determine the gas separation performance. Beyond the measurement of these properties, molecular dynamics simulations could provide deeper insight into the gas transport mechanism, and the relationship between structure and properties.Incorporating spacer such as triptycene moieties into amorphous polymers (PIM: polymers with intrinsic microporosity) has led enhanced permeability and selectivity. This is assumed to be achieved by effective blocking of polymer chain packing, thereby increasing the free volume inside the polymer membrane to improve gas transport properties.In this study, we clarified the origin of such improvement with the density, fractional free volume (FFV), x-ray diffraction (XRD) pattern, solubility, diffusivity, permeability, and selectivity calculated by molecular dynamics simulations. As a model system, polybenzoxazole membranes having triptycene spacers with varying ratio were selected.

Poster Presentation : **PHYS.P-253**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Ligand Field Effect at Oxide-Metal Interface on the Dissociation of an O_2 Molecule on Ultrathin MgO/Ag(100) Surface

Prihatno Fajar, Jaehoon Jung[*]

Department of Chemistry, University of Ulsan, Korea

Controlling the chemical reactivity for O_2 dissociation as an elementary step is of importance in a broad range of chemical reactions. Here we investigate the influence of first-row transitional-metal dopant on the dissociation of O_2 adsorbed on ultrathin MgO film grown on Ag(100), using periodic density functional theory (DFT) calculations. The adsorption and dissociation of O_2 are strongly dependent on the spin state of oxygen atoms on the surface, which is closely related to the charge transfer and adhesion strength due to the kind of transition metal dopant. We found that the dissociation of O_2 molecule leads to the formation of one negative oxo ion and one neutral oxygen atom on MgO surface. In addition, the magnetization and atomic charge of dissociated products on the doped 2-ML MgO/Ag(100) show a double-humped pattern which can be interpreted with ligand field stabilization energy (LFSE) at the oxide-metal interface. Our computational study provides not only profound insight into chemical reactivity control of ultrathin oxide film supported by a metal substrate but also an impetus for investigating ultrathin oxide films for a wider range of applications.

Poster Presentation : **PHYS.P-254**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Local mapping of ultrafast carrier/exciton dynamics with transient absorption microscopy

Won-Woo Park, Oh-Hoon Kwon*

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

Transient absorption (TA) spectroscopy has drawn great attention for examination of the carrier/exciton dynamics in solar cell[1], valleytronics[2], and photocatalytic[3] materials because of its sensitivity to both dark and luminescent states, high temporal resolution, and broadband probe range. With the continuing development of electronic materials, the necessity to understand the effect of microscopic heterogeneity and morphology of materials on its exciton/carrier dynamics has encouraged the development of microscopic study of TA.TAM technique, combining the conventional TA spectroscopy with the optical microscopy, retrieves the shortcoming on the spatial resolution of the TA spectroscopy and opens a new field for the investigation of morphological and structural dependence of photoinduced dynamics. Here, we visualize the TAM technique, which has ultrashort time resolution (~100 fs) and broadband probe ranges (400–1500 nm) with a spatial resolution of 5 μm, and demonstrate its capability of spatial resolution with the novel optoelectronic material, WS_2. By resolving the transient absorption spectra of WS_2 flakes in both time and space, thickness-dependent and site-specific photoinduced dynamics is demonstrated. References[1]T. H. Lee, W.-W. Park, S. Y. Park, S. Cho, O.-H. Kwon and J. Y. Kim, Solar RRL 5, 2100326 (2021).[2]H. Zhou, Y. Zhao, W. Tao, Y. Li, Q. Zhou, and H. Zhu, ACS Nano 14, 4618-4625 (2020).[3]F. V. A. Camargo, Y. Ben-Shahar, T. Nagahara, Y. E. Panfil, M. Russo, U. Banin, and G. Cerullo, Nano Lett. 21, 1461-1468 (2021).

Poster Presentation : **PHYS.P-255**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Dry plasma reduction to fabricate gold nanoparticle on cellulose paper as broadband plasmonic absorber

Trinh Ba Thong, Kwanghyeon Jo, Deun Chan Lee, Ilsun Yoon*

Department of Chemistry, Chungnam National University, Korea

Efficient solar energy harvesting of plasmonic absorbers play an important role for many applications. Here, we demonstrate a simple method of depositing the AuNPs on cellulose filter paper using dry plasma reduction (DPR) under atmospheric pressure and low temperature to form the black plasmonic AuNPs paper (BPAP). The surface morphology of BPAP can be controlled by optimizing the synthesis condition, such as plasma power and the precursor concentration, and characterized by using transmission electron microscopy (TEM). The BPAP substrate shows the broadband solar absorption up to 93% in the wide spectral range (350 to 1800 nm, AM 1.5G), with maximum absorption of 98.4% in the visible region and the minimum absorption of 79.3% in the near-infrared region. With the simple fabrication method and high efficient solar energy absorption, the BPAP substrate will be a promising plasmonic absorber for many photothermal conversion application.

Poster Presentation : **PHYS.P-256**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

A facile synthesis and time-resolved fluorescence studies of P3HT crystalline particles

MinHee Lee, Seung Jin Jung, YouMin Park, Jaehong Park*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Conjugated-polymers in condensed-phase have different optoelectronic characteristics depending on their morphology and these properties affect device performance. We produced highly crystalline P3HT particles (P3HT-CPs) using an antisolvent slow-diffusion method. The particle dimensions of P3HT-CPs ranging from 100s ns to a few microns were observed through SEM images. The XRD and TEM characterization results of P3HT-CPs proposed a highly-ordered packing consisting of P3HT backbones along the (100) direction and markedly suppressed amorphous fractions. We utilized time-correlated single-photon counting (TCSPC) experiments to figure out fluorescence lifetime of intrinsic exciton of P3HT-CPs. The optical spectroscopic results, including absorption spectra and TCSPC analysis will be discussed.

Poster Presentation : **PHYS.P-257**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Photoinduced carrier-dynamics of non-fullerene acceptor-based P3HT-NDI block copolymer self-assembly

YouMin Park, So-Jung Park*, Jaehong Park*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Non-fullerene acceptors have been adopted in various optoelectronic applications, including photovoltaics due to their bandgap tunability, enhanced extinction coefficient with respect to fullerene. Here, we prepared the self-assembly of a block-copolymer (P3HT-NDI), possessing an electron-donor (P3HT) and a non-fullerene electron-acceptor (naphthalene diimide, NDI), using the Air-Liquid Interfacial Assembly (ALISA) method. NMR, GPC and TEM characterization results of the P3HT-NDI block copolymer as well as the P3HT-NDI self-assembly suggest not only well-synthesized block copolymer formation consisting of P3HT and NDI, but also aligned nanoarrays, featuring the well-ordered packing through the π-π and backbone-backbone interactions between P3HTs. We utilized flash-photolysis time-resolved microwave conductivity (FP-TRMC) experiments to explore the carrier dynamics of the P3HT-NDI self-assembly. Flash Photolysis Time-resolved Microwave Conductivity (FP-TRMC) is an electrodeless photoconductivity measurement which can figure out carrier information like carrier generation yield (ϕ), mobilities ($\sum\mu = \mu_e + \mu_h$, the sum of electron/hole mobilities), and recombination dynamics. The optical spectroscopic results and $\phi\sum\mu$ transients data will be discussed.

Poster Presentation : **PHYS.P-258**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Real-time observation of nucleic acid unwinding process by SARS-Coronavirus Nsp13 at single-molecule level

Hyunggi Kim, Dong-Eun Kim[1], Hye Ran Koh*

Department of Chemistry, Chung-Ang University, Korea

[1]*Department of Biotechnology, Konkuk University, Korea*

The Severe Acute Respiratory Syndrome Coronavirus (SARS-CoV) helicase, non-structural protein 13 (nsp13), unwinds double-stranded RNA (dsRNA) starting from the 5’ tail of single-stranded RNA (ssRNA) to 3’ direction in an ATP-dependent manner. Nsp13 helicase plays a crucial role in RNA replication by separating dsRNA, contributing to the reproduction of viral RNAs. Therefore, it is indispensable to unveil the molecular mechanism of dsRNA unwinding by nsp13 to understand the virus life cycle, but it still remains elusive. To discover the molecular mechanism of dsRNA unwinding reaction by nsp13, we employed single-molecule fluorescence resonance transfer, which enabled to track the unwinding process in real time. Interestingly, we found that nsp13 experienced the multiple rounds of partial unwinding proceeding the complete unwinding of dsRNA. In addition, the several intermediate states were observed during the unwinding process, suggesting that dsRNA unwinding process by nsp13 is a multi-step process. We also investigated the kinetic steps of dsRNA unwinding by nsp13, revealing that nsp13 unwound dsRNA with a 3 bp unwinding step size.

Poster Presentation : **PHYS.P-259**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

FTIR, 2D IR, and computational studies of two coupled C=O stretching modes of xanthine and its derivatives in aqueous solution

Jin Gyu Seol, Hyejin Kwon, Yung sam Kim*

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

Xanthine can be obtained during the purine metabolism reaction, and a large amount of xanthine in the human body may cause kidney stones. Xanthine derivatives are easily observed in coffee or chocolates, which are heavily consumed in the human body. Therefore, the molecular property and dynamics of xanthine and its derivatives in an aqueous solution is a topic of considerable interest. Xanthine and xanthine derivatives (theobromine, theophylline, paraxanthine, and caffeine) have two adjacent carbonyl groups, making them good candidates to study by infrared spectroscopy. However, infrared studies of xanthine in an aqueous solution have not been reported because of the low water solubility of xanthine. In this regard, two-dimensional infrared (2D IR) spectroscopy, which has the effect of suppressing the background signal, was used to detect a weak sample signal. In parallel, *ab initio* calculation was also performed for the xanthine in an aqueous solution. FTIR, 2D IR, and computational studies of xanthine and xanthine derivatives in D_2O solutions are presented in this work.

Poster Presentation : **PHYS.P-260**

Physical Chemistry

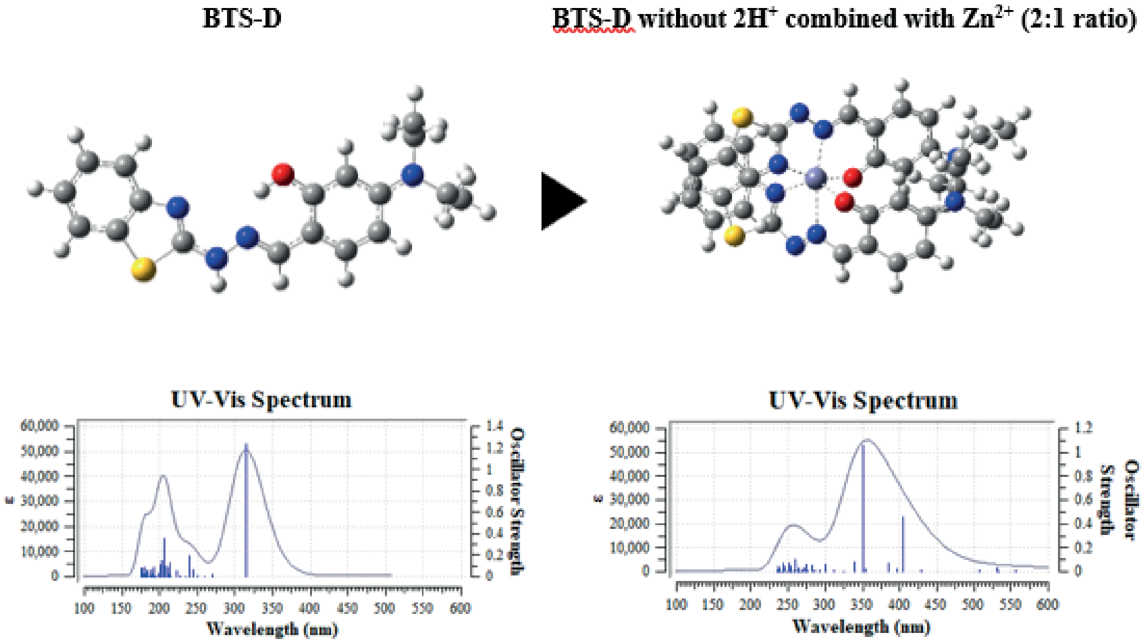
Exhibition Hall 1 THU 11:00~12:30

DFT/TD-DFT study of benzothiazole derivative chemosensors for the detection of Zn2+ via intramolecular charge transfer sensing strategies

Jong-Won Song[*], **Yeonggil Seo**[1]

Chemistry Education, Daegu University, Korea
[1]*Chemistry education, Daegu University, Korea*

Our collaborator recently designed benzothiazole derivatives (BTS-D and BTS-W) which are fluorescent chemosensors over Zn2+ metal ion in aqueous samples with 2:1 stoichiometric ratio (probe: Zn2+). In order to clarify the structures of BTS-D and BTS-W binding with Zn2+, we performed quantum chemical calculations using long-range corrected (LC) density functional theory (DFT) and time-dependent (TD) DFT. We confirmed that the structures showing the best binding energies with Zn2+ by 2:1 ratio reproduced the experimental UV-vis spectra, which presents that LC-DFT is a useful quantum chemical method for elucidating the structure of chemosensor as well as its photochemical mechanism. In addition, our quantum chemical study clarifies that the Zn2+ binds with hydroxyl oxygen, imine nitrogen, and benzothiazole nitrogen of each probe as a hexagonal complex in both BTS-D and BTS-W.



BTS-D

BTS-D without $2H^+$ combined with Zn^{2+} (2:1 ratio)

Poster Presentation : **PHYS.P-261**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effect of the abolition of intersubunit salt bridges on allosteric protein structural dynamics

Minseo Choi, Hyotcherl Ihee[1,*]

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

As one of the representative structural factors established by non-covalent interactions, salt bridges play an important role in stabilizing structure and regulating protein function, but their role in dynamic processes is veiled. We investigated the effect of salt bridges on the allosteric structural transition of homodimeric hemoglobin (HbI) by applying time-resolved x-ray solution scattering (TRXSS) to the K30D to scrutinize the structural and functional roles of salt bridges in the process of performing protein functions. The TRXSS data of K30D, a mutant with abolished interfacial salt bridges of the wild-type,[1] describes a kinetic model that requires one monomer intermediate in addition to the three structurally distinct dimer intermediates (I1, I2, and I3) observed in WT and other mutants.[2] Kinetics and structural analyzes reveal that salt bridges interfere with the R-T allosteric transition of HbI by showing that K30D has more than nine times accelerated transition from I2 to I3 compared to WT and no significant structural changes observed in the transition from R-like I2 to T-like I3 observed in WT. Moreover, the correlation between the rates of bimolecular CO recombination in K30D, WT and other mutants indicate that bimolecular CO recombination is abnormally slowed in K30D, indicating that salt bridges also affect cooperative ligand binding of HbI. These comparisons of the structural dynamics and kinetics of K30D and WT shows that the interfacial salt bridge not only supports the physical connection of the two subunits but also plays an important role in the global structural signal transduction of one subunit to the other subunit through a series of well-organized structural transitions.

Poster Presentation : **PHYS.P-262**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Molecular dynamics study of anomaly in nano-confined water

Youngji Jeong, Chang yun Son*

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

Water for us is so near and yet so far to be fully understood. Studying unique nature of water, nanometer-size confined water is one of the unresolved problem as its properties differ from bulk water. Both experiments and simulations proposed unusually low dielectric constant of water under confined system. Polarization effect and anisotropic dipole correlation are given for the reason. Still, reducing factor of dielectric constant of confined water is unclear. Another example of structural anomaly in nano-confined water can be found in the highly-debated square ice, which was observed to be stabilized under extreme confinement between high pressured graphene sheets. In this study, we conducted molecular dynamics (MD) simulations of nano-confined water, focusing on the effect of dielectric boundaries. Recently developed simulation method enabled us to systematically control the effect of surface polarization and molecular polarization, along with geometric constraints imposed by different wall boundary conditions and the size of confinement.Simulations revealed that confined water consistently showed lower dielectric constant than the bulk regardless of the characteristics of confining surface, while the extent of reduction in dielectric response strongly depended on the dielectric property of confining walls. Remarkably, the confinement-induced lower dielectric response persisted up to multiple tens of nanometers, raising questions on the traditional explanation relying on the model of a-few layer thick surficial water and bulk-like water layer. Furthermore, MD simulations under extreme confinement of sub-nanometer sized confinement showed several highly ordered structures, where both the structure and dynamics of them showed intriguing dependence on the molecular defect existing due to the finite sized slab.As simulation can control certain physical properties artificially, further exploring is going to be done to find out how interfacial alignment, electrostatic properties, and the existence of external electric field changes the dynamics. It will allow us to discover the origin of such anomalies.

Poster Presentation : **PHYS.P-263**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Plasma induced AuNP reduction on cellulose paper and SERS application

Kwanghyeon Jo, Rashida Akter, Trinh Ba Thong, Ilsun Yoon[*]

Department of Chemistry, Chungnam National University, Korea

Surface enhanced Raman scattering (SERS) is a powerful detection technology apply in various fields such as discrimination of drugs, contaminants, and spoiled food, with high sensitivity and selectivity. The enhancement is strongly contributed by the light-induced electric field in the space between the metallic nanostructured. Here, we demonstrate an in-situ fabrication method to growth the gold nanoparticles with small nm gap on the cellulose filter paper using dry plasma reduction (DPR) process. The substrate with lots of small nm gap between the AuNPs shows the high extinction in the NIR region. A finite-difference time-domain (FDTD) simulation was also employed to investigate the electric fields distribution of the substrate. This AuNP-cellulose substrate shows a SERS enhancement factor of ~ 5×10^6, and a relative standard deviation (RSD) of 9.1% over an area 50×50 μm^2 using 1,4 benzene thiol as the Raman reporter. With the simple synthesis process and good sensitivity, it is anticipated that the cellulose-based SERS will be applicable not only for chemical detection, but other application like biosensor or environmental monitoring.

Poster Presentation : **PHYS.P-264**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

[Withdrawal] Observation of the charge transfer induced structural dynamics at the photoexcited gold-TiO_2 bilayer thin film

Jun Heo, Hyotcherl Ihee*

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

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **PHYS.P-265**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

[Withdrawal] Reactive laser ablation of Ti in oxygen atmosphere

<u>Dong Hun Hwang</u>, Jae Kyu Song, Seung Min Park[*]

Department of Chemistry, Kyung Hee University, Korea

Poster Presentation : **PHYS.P-266**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Quantum Chemical Calculations of binding energy of MnCl2 with Cycylodextrin/graphene using B3LYP-D3 functional

Hwiseo Kim, **Jong-Won Song***

Chemistry Education, Daegu University, Korea

- Withdrawal -

Poster Presentation : **PHYS.P-267**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Active site fortification in Dual-Phase Nickel Sulfide Nanospheres by Cation Modulation using Pulsed Laser Irradiation: Overall Water Splitting and Methanol Oxidation Reaction evaluation

Deviprasath Chinnadurai, Myong Yong Choi[1,*]

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

Nickel-based sulfides, oxides, selenides occupy the most important place when it comes to the transition metal-based electrocatalyst. In this study, we used an extremely effective controllable pulsed laser irradiation (PLI) technique to fabricate dual-phase nickel sulfide, and we enhanced the catalytic activity cation modulation using Co and Cu atoms. Electrochemical performances of oxygen evolution reaction (OER), hydrogen evolution reaction (HER), and methanol oxidation reaction (MOR) measured in an alkaline medium proves the multifunctional activity. The cation adjustment resulted in the improvement of the catalytic performance of HER and OER during Cu and Co substitution, respectively. For the Co-Ni-S sample in OER, we achieved an overpotential of 368 mV at 10 mA/cm2 in OER. The higher ECSA Cu-Ni-S sample improved HER activity at a lower overpotential of 271 mV at 10 mA/cm2 and a lower Tafel slope of 98 mV/dec. The excellent bifunctional activity enhanced overall water splitting with a lower voltage of 1.88 V to achieve a geometrical current density of 10 mA/cm2, with high durability. Meanwhile, the high selectivity of Cu resulted in a very high methanol electrooxidation activity with a current density as high as 55.4 mA/cm2. The detailed electrochemical studies were presented with their supporting physiochemical analysis. This report shows the efficiency and simplicity of fabricating transition metal derivatives and cation modulation using superficial laser methods.

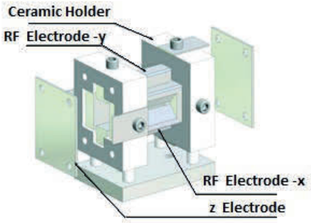
Poster Presentation : **PHYS.P-268**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

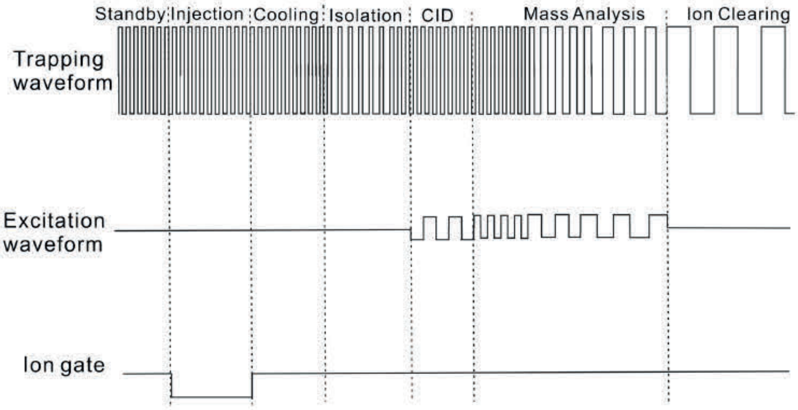
Building a Miniature Digital Rectilinear Ion Trap Mass Spectrometer

Md Musleh Uddin Munshi[*], **Han Bin Oh**[*]

Department of Chemistry, Sogang University, Korea

We aim to build a miniaturized digital rectilinear ion trap (DRIT) mass spectrometer (~10x10x40 mm3) (Fig 1). Incorporation of digital technology in ion trap (Paul type, linear quadrupole) MS is not new. Recently, this got the most attention due to the advancement of digitization. We have already designed and manufactured the RIT based on the existing design of Ouyang et al. These RITs have geometries that are much simpler than hyperbolic Paul traps which enable tremendous control to manufacture. In addition, RITs show much higher trapping capabilities. Crucial advantage of the RIT based mass analyzers is the use of digital rectangular waveforms on the electrodes instead of classical rf-Sine waveforms. Besides, the mass scan is achieved by frequency scan while the voltage is held constant but not the opposite. Manipulation of the duty cycle of the trapping waveform and the excitation waveform allow us to carry out mass (m/z) isolation and CID MS respectively without the need of additional circuitry. Not to mention, RITs require much lower voltage (~600 Vp-p) to operate than Paul traps which helps to avoid electrical discharge. In this research, we employ commercially available software SIMION/SIMAX for simulation of ion motions inside RIT. This theoretical study will allow us to optimize crucial parameters further to build the instrument. //Fig 1. RIT assembly and the schematic of the experimental timing sequence adopted from Ouyang et al, and Xu et al respectively. //References:(1)Richards et al, IJMS, 1973, 12, 317-339(2)Ding et al, 2002, 221, 117-138(3)Ouyang et al, Anal. Chem. 2004, 76, 16, 4595-4605(4)Ding et al, J. Mass Spectrom, 2004, 39, 471-484(5)Xu et al, J. Am. Soc. Mass Spectrom. 2014, 25, 556-562(6)Ding et al, Analyst, 2016, 141, 5535


Ceramic Holder
RF Electrode -y
RF Electrode -x
z Electrode


Standby
Injection
Cooling
Isolation
CID
Mass Analysis
Ion Clearing
Trapping waveform
Excitation waveform
Ion gate

Poster Presentation : **PHYS.P-269**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Wettability of multi-layered graphene and interfacial water structure revealed by VSFG

Eunchan Kim, Minhaeng Cho*

Department of Chemistry, Korea University, Korea

Understanding of water interacting with multi-layered graphene is important for a variety of applications such as desalination, energy storage, and catalysis. However, the hydrogen-bonding(H-bonding) structure of water at the graphene-water interface has been poorly studied. Vibrational sum-frequency-generation (VSFG) spectroscopy is suited to investigate H-bonding structure at graphene-water interfaces. Stacking the graphene layer, the interfacial water structure changes depending on the number of graphene layers. Dangling OH groups which do not interact with other water molecules become increasingly apparent as the number of graphene layer increases. The fraction of dangling OH groups inferred from the VSFG spectrum correlates with the water contact angle results. Our observation suggests that VSFG could be an useful technique for measuring the water adhesion energy on any spatially confined interface where the water contact angle cannot be measured. We anticipate that VSFG spectroscopy could shed light on the wettability of 2D-materials.

Poster Presentation : **PHYS.P-270**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Wavefront controlled coherent anti-Stokes Raman scattering microscopy

Youngjin Choi, Jong Min Lim[1,*], Minhaeng Cho[1,*]

Korea University, Korea

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

The wavefront correction system, also known as CLASS (Closed Loop Accumulation of Single Scattering), was introduced into the CARS microscopy to obtain a tightly focused beam even under severe aberration sample conditions. Based on the label-free strength of a CARS microscopy, over the past decade, the CARS microscopy has been used to discover the chemical environment and characteristics of biological samples. However, when the focus of light is affected by deep observations or the presence of opaque structures such as bones, the CARS signal is further reduced non-linearly. Here, the CLASS system was applied to the CARS microscopy to investigate biomolecules in deeper penetration depth and in-vivo. With wave correction function of adaptive optics, the beam has also been closely re-focused on aberration materials. We first demonstrated our system's aberration correction capability with artificial targets. Next, the myelins present in the mouse brain were observed at a deep depth and in-situ state without skull removed.

Poster Presentation : **PHYS.P-271**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Substituent Effects on the Vibrational Properties of the CN Stretch Mode of Aromatic Nitriles: IR Probes Useful for Time-resolved IR Spectrsocopy

Suin Choi, Kyungwon Kwak[1,*], Minhaeng Cho[1,*]

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

It is essential to investigate the ultrafast structural and dynamics of biomolecules like peptides and proteins since information on changes in the structure of biomolecules can determine their functions and properties. Time-resolved IR spectroscopy is well suited for observing protein structure and dynamics owing to its inherently fast timescale. However, since biomolecules such as peptides and proteins are composed of various amino acids connected through multiple intermolecular and intramolecular interactions, their IR spectra are spectrally complex and entangled. These challenges have been solved through the development of IR probes which can be introduced on a specific position in biomolecules. Especially, the nitrile (CN) group is one of the very first side chain-based IR probes to study the local environment of proteins. Herein, we investigated the effect of a substituent on the vibrational properties of the benzonitrile. The electron-donating and withdrawing character of p-substituent on benzonitrile are expected to modulate the vibrational frequency, molar extinction coefficient, and vibrational lifetime. FT-IR revealed the positive correlation between electron-donating character and the molar extinction coefficient of CN stretch mode. Infrared pump-probe (IR-PP) measurements showed that the vibrational lifetime of CN stretching mode exhibits a relatively weak correlation with the electron-donating strength. Among the investigated samples, 4-dimethylamino benzonitrile with the strongest electron-donating strength exhibits enhanced absorption and extended vibrational lifetime. Utilizing substituent effects will be a practical strategy to improve the performance of the IR probe.

Poster Presentation : **PHYS.P-272**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Accurate prediction of optical properties of organic molecules by deep learning optical spectroscopy

Minhi Han, Min Seok Jeong, Sungnam Park[1,*]

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

Deep learning has been successfully used in chemistry for a variety of purposes, such as toxicity, reactivity, solubility, reaction mechanism, synthetic pathway, and chemical and physical properties. Although deep learning has potential in many research areas, its practical applications in chemistry are limited largely due to a lack of a sufficiently large database. In this work, we have built an experimental dataset of various optical properties of more than 60k chromophore/solvent combinations by collecting them in the literature. In addition, we have developed a deep learning optical spectroscopy (DLOS) to accurately predict various optical properties of organic chromophores in various environments, such as absorption and emission maximum wavelengths and their bandwidths (full width at half maximum), molar extinction coefficient, photoluminescence quantum yield, and fluorescence lifetime. The solute-solvent interactions are included in our DLOS such that the solvatochromic shift, aggregation induced emission, and other solvent-dependent properties are well predicted. The results of our DLOS will be presented.

Poster Presentation : **PHYS.P-273**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

DFT Functional Dependency on Graphene-Related Materials

Youngsam Kim, Suhwan Song, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

Graphene is one of the most popular materials in solid-state chemistry. The properties of pristine graphene have been well studied and are of interest for many applications. Computational chemistry has also contributed significantly to the study of these applications. Due to its practical cost and sufficiently accurate results, density functional theory (DFT) is the preferred choice for electronic structure calculations. However, the exact exchange-correlation (XC) functional is not yet known, and the approximate manners cause the approximate functionals to have their own dependencies on the system. In particular, semi-local functionals often fail to predict long-range interactions, a key characteristic of adsorption processes, and these defects are highly system-dependent. Here, we discuss the XC functional dependency on graphene-related materials by comparing the optimized structure and the electronic structure.

Poster Presentation : **PHYS.P-274**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Constrained Unrestricted Hartree-Fock Based Double-Hybrid Density Functional Approximation: cuBL1p

Hayoung Yu, Suhwan Song, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

Density Functional Theory (DFT) is one of the popular methods which is able to calculate electronic structures of organic, inorganic, and material systems with reasonable computational cost. However, for reactions such as reaction barrier heights, bond formation and breaking, and reactions including transition states, standard DFT suffer not only from the inaccurate approximation of the exchange-correlation potential but also from the errors from self-consisted density. To handle this problem, one of the practical ways is adopting a non-self-consistent way based on the Hartree-Fock (HF) density to deal with density-driven error, called HF-DFT. Most recently, the BL1p method is introduced in [J. Phys. Chem. Lett. 12, 800 (2021)] which is the double-hybrid method based on the HF density. The performance of BL1p is comparable to the other highly parametrized functionals but, due to the HF scheme, it suffers from spin-contamination and, for large spin-contaminated cases, the BL1p result becomes unreliable. Here, we introduce the cuBL1p method which is the same XC functional to the BL1p but based on the Constrained Unrestricted HF formalism. Unlike BL1p, cuBL1p doesn't suffer from spin-contamination by definition while its performance is as good as BL1p.

Poster Presentation : **PHYS.P-275**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Structural transformation of N-doped graphene sheet adsorbed at Metal surface

Muthu Austeria Prem Kumar, Do hwan Kim[1,*]

Nano convergence engineering, Jeonbuk National University, Korea
[1]*Department of Chemistry Education, Graduate School of Department of Energy Storage/Conversion Engineering, Jeonbuk National University, Korea*

Ab-initio calculations have been performed to study the geometry and electronic structure of nitrogen (N) doped graphene sheet on metal surface. The effect of doping has been investigated by varying the concentrations of N and also by considering different doping sites at the metal surface. All the calculations have been performed by using VASP (Vienna Ab-initio Simulation Package) based on density functional theory. While the planar structure of the graphene sheet affected on N doping which is adsorbed to the metal surface, Moreover the concentration of N dopant at graphene determines the non-planarity. N connected on metal surface induces non-planarity than C-connected metal surface. The partial transformation sp2 to sp3 carbon identified with chair formation at six membered ring. These interesting results provide the possibility of tuning the band gap of graphene adsorbed metal surface and in-depth studies for the inorganic/organic surface interaction are required for energy related applications.[Acknowledgement] This research was supported by the Regional Leading Research Center Program (2019R1A5A8080326) through the National Research Foundation funded by the Ministry of Science, and ICT and Future Planning of the Republic of Korea.

Poster Presentation : **PHYS.P-276**

Physical Chemistry

Exhibition Hall 1 THU 11:00~12:30

Comprehensive computational study on the surface of oxygenated di-nickel di-selenide for hydrogen evolution reaction

Prabhakaran Sampath, Do hwan Kim[1,*]

Department of Nano Convergence Engineering, Jeonbuk National University, Korea

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

Seeking high-performance and low-cost electrocatalysts is of great importance for energy-saving and green hydrogen generation. Hereby the surface phenomena of O-Ni2Se2 were investigated with density functional theory (DFT) calculations simulated with GGA-PBE and Grimme's DFT-D3 functions. These comprehensive designs were theoretically examined with an appropriate catalyst that outperforms with high energy barrier and shows the density of states (DOS) with higher conductivity around Fermi level and lower Gibbs free energy ΔGH=0.3029eV towards HER.This research was supported by the Regional Leading Research Center Program (2019R1A5A8080326) through the National Research Foundation funded by the Ministry of Science, and ICT and Future Planning of the Republic of Korea.

Poster Presentation : **PHYS.P-277**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Machine-Learned XC Functional with Decomposed Error Target

Sechan Lee, Suhwan Song, Eunji Sim[*]

Department of Chemistry, Yonsei University, Korea

In modern computational chemistry, Kohn-Sham Density functional theory (KS-DFT) is the standard method for theoretical studies of the properties of molecules. However, the practical KS-DFT has the error called total error from the exact KS-DFT cause the exchange-correlation (XC) functionals are approximated. The total error can be decomposed into two components: density-driven error and functional error. Due to these two types of error, describing the physical properties is difficult when the XC functionals are made up by targeting the total error. These XC functionals are suffered from the mixed effect of density-driven and functional error, but by targeting each error separately or together, you can more intuitively understand the meaning of the errors of functionals. In this presentation, the machine learning technique is used to create an XC functional that targets decomposed errors for the flexibility of the functionals.

Poster Presentation : **PHYS.P-278**

Physical Chemistry

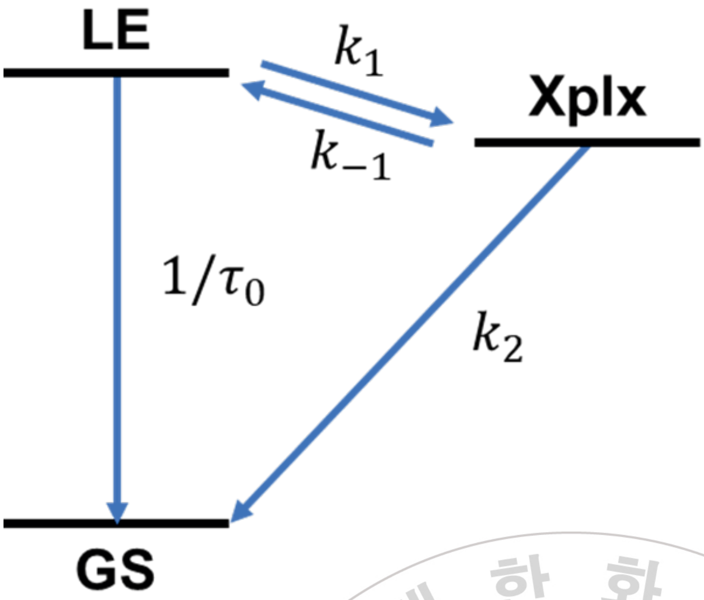
Exhibition Hall 1 THU 11:00~12:30

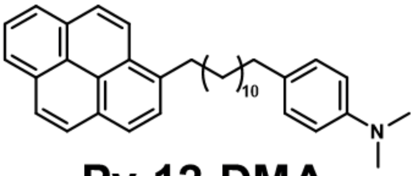
Kinetic Study of Chain-linked Electron Acceptor / Donor System in Non-polar Solvent

Dongcheol Park, Hohjai Lee[1,*]

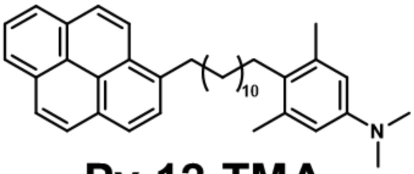
Department of chemistry, Gwangju Institute of Science and Technology, Korea
[1]*Chemistry, Gwangju Institute of Science and Technology, Korea*

Unlike the freely diffusing exciplex-forming electron donor (D) and acceptor (A) system whose kinetic heavily depends on the diffusion and their concentration, the exciplex-forming chain-linked A/D system provides unique physical properties such as efficient excitation quenching process, high quantum yield of exciplex, and prolonged spin correlation time. The chain-linked D-A system is also practically superior in that it requires low concentration, as low as 10 μM. In this poster, we propose a kinetic model for chain-linked A/D system in non-polar solvent, a simple system that does not generate radical ion pair. The model is composed of three states: a locally excited state (LE) in which acceptor moiety is photo-excited from the ground state (GS), and an exciplex (Xplx) generated by photo-induced electron transfer from LE. In the kinetic model, LE has relaxation process to GS ($1/\tau_0$) and electron transfer process to Xplx (k_1), and Xplx has back electron transfer process to LE (k_{-1}) and relaxation to GS (k_2). We have synthesized and studied two chain-linked A/D samples (pyrene-$(CH_2)_{12}$-N,N-dimethylaniline, Py-12-DMA, and pyrene-$(CH_2)_{12}$-N,N,3,5-tetramethylaniline, Py-12-TMA) that have different oxidation potentials to verify kinetic model and to demonstrate its generality. Also, 1-dodecylpyrene (Py-12) was synthesized as a control. To obtain kinetic values LE, Xplx, and Py-12 lifetime were measured using by TCSPC. The total electron transfer rate ($k_{et} = k_1/(1+k_{-1}/k_2)$) from the time-resolved spectroscopic measurements were crosschecked with one obtained from the quantum yield measurement.

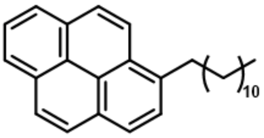




Py-12-DMA



Py-12-TMA



Py-12

Poster Presentation : **PHYS.P-279**
Physical Chemistry
Exhibition Hall 1 THU 11:00~12:30

Long-range corrected exchange-correlation functional including a two-Gaussian Hartree-Fock attenuation for core-excited-state calculations of second-and third-row atoms (LC2gau-BOP)

Hanseok Bae , Jong-Won Song[1,*]

Chemical education, Daegu University, Korea
[1]*Chemistry Education, Daegu University, Korea*

Previously, we presented improved long-range corrected (LC) density functional theory (DFT) schemes, named “LCgau” [J.-W. Song et al., J. Chem. Phys. 129, 184113 (2008)] and “LC2gau” [J. Chem. Phys. 131, 144108 (2009)]. By introducing a flexible mixing of Hartree–Fock and DFT exchange in the LCgau scheme, we showed that a DFT functional could simultaneously achieve high accuracy in the reproduction of core excitations of 2nd-row atoms (C, N, O, and F atoms), as well as charge transfer and valence-Rydberg excitation energies. In this research, we will show that with a flexible mixing of two-Gaussian short-range exchange, LC2gau can reproduce core excitations of both the 2nd- and 3rd-row atoms simultaneously with high accuracy. It will be presented that LC2gau can simultaneously perform well for all types of excitations, as well as thermochemistry. A notable feature is the flexible inclusion of a short-range Hartree-Fock exchange can improve the performance of DFT functional for various kinds of orbital energy calculations.

Poster Presentation : **ANAL.P-191**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Analytical method for parabens in water using LC-MS/MS and GC-MS/MS

In ja Lee

Seoul Water Institute, Korea

In order to analyze the concentration of parabens in a water sample, a reliable analysis method capable of measuring up to a concentration level of several ng/L is required. In this study, four types of parabens(Methylparaben, MP; Ethylparaben, EP; Propylparaben, PP; Butylparaben, BP) were analyzed using liquid chromatography tandem mass spectrometer (LC-MS/MS) and gas chromatography tandem mass spectrometer (GC-MS/MS). LC-MS/MS equipped with online solid-phase extraction(SPE) was used and analyzed using a Poreshell 120 EC (2.7 µm; 3.0 mm × 50 mm) column. The calibration curves showed good linearity with high correlation coefficients (>0.996) excluding MP. The method detection limits (MDL) and the limit of quantification (LOQ) were 1.5 to 3.0 ng / L and 4.9 to 9.5 ng / L, respectively. Samples applied to GC-MS/MS were pretreated with a solid phase extraction device using a HLB (Hydrophile-liphophile balance) cartridge, and then analyzed using a DB-5MS column. The calibration curves showed good linearity with high correlation coefficients (>0.996) excluding methylparaben. The MDL and LOQ were 0.8-1.2 ng / L and 2.5-3.8 ng / L, respectively.

Poster Presentation : **ANAL.P-192**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Identification of tire road wear particles generated from passenger vehicles

Eunji Chae, Sung-Seen Choi[*]

Department of Chemistry, Sejong University, Korea

Various particles are presented on the road, such as wood, glass, stone, worn road pavement, and abraded tire tread. These particles can flow into rivers, lakes, and seas by rainwater or runoff, causing marine pollution. And they may become a cause of air pollution by floating in the atmosphere. Besides, if they enter the human body, it can harm cardiopulmonary health. Particles produced from the vehicle's non-exhaust include tire wear particles, brake wear particles, and road wear particles. Wear particles are generated by the contact and friction between the road and tires. In general, it exists as tire road wear particles (TRWPs) which road wear particles are attached to tire tread wear particles. Since kinds of rubbers used for passenger car and bus tires are different, the source of tire wear particles can be determined by analyzing rubber composition of a single TRWP. We collected road dust near the taxi stand to study the TRWP generated by passenger car tires. Kinds of cured rubbers such as tire treads are typically analyzed using pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS). Py-GC/MS can analyze without sample pretreatment and can analyze a small amount of sample. Characteristic pyrolysis products differ depending on kinds of rubber. For example, the main pyrolyzates of styrene-butadiene rubber (SBR) are butadiene, 4-vinylcyclohexene, and styrene. In this study, we analyzed rubber composition of a single TRWP produced on the road and their sources were investigated.

Poster Presentation : **ANAL.P-193**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Determination of inorganic arsenics by capillary ion column

Seon-jin Yang, Sang-Ho Nam*, DongChan Lee, Yonghoon Lee

Department of Chemistry, Mokpo National University, Korea

The toxicity and biological activity of arsenic depends on chemical forms or species. In particular, the inorganic arsenics are more toxic than the organic arsenics. Thus, the accurate determination of arsenic species is important. A method of separating arsenic species using a cation and an anion separation column has been widely used. The conventional columns typically use the sample loops with a volume of 100-1000 µL. The amount of samples required for analytical measurements should be at least three times the volume of the sample loop. However, it is difficult to apply to limited samples such as clinical and biological samples.In this study, we investigated a capillary column with a small sample loop of 5 µL for the separation of arsenic species. The standard solutions of DMA, MMA, As^{3+}, and As^{5+} were prepared, and the inorganic arsenic and organic arsenic were separated using a capillary column. The separated arsenics were determined by inductively coupled plasma mass spectrometry (ICP-MS). The linear calibration curves from 0.5 µg/kg to 25 µg/kg were obtained for inorganic arsenic, the correlation coefficient was 0.9999. The recovery efficiency of a standard 20 µg/kg inorganic arsenic was 100 %. Inorganic arsenic was determined in NIST water CRM 1643f to validate the analytical method. The recovery of inorganic arsenic was 101 %.

Poster Presentation : **ANAL.P-194**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Characteristic analysis of natural rubber wear particles depending on the particle size by the shapes and pyrolysis products

Uiyeong Jung, Sung-Seen Choi*

Department of Chemistry, Sejong University, Korea

Various wear particles are generated by friction between tires and the road. These wear particles are present as road dust. The particles float in the air and cause air pollution as fine dust or enter the aquatic environment through sewers to cause water pollution. Tire wear particles are classified as microplastic and are considered as one of major environmental pollutants. Thus, many studies on tire wear particles are in progress. Tires are made of rubber and various additives. In particular, bus and truck tire treads mainly use natural rubber (NR). In the present work, we characterized NR wear particles depending on the size by the shapes and pyrolysis products. A model NR compound was prepared, NR wear particles using a laboratory abrasion tester (LAT), and they were separated by size using a sieve shaker. Among them, the wear particles of above 63 μm were used for analysis. The shapes of the wear particles were analyzed with an image analyzer. The shapes were classified into linear, branched, curved, and others types. A single wear particle was pyrolyzed and the pyrolysis products such as isoprene and dipentene were analyzed. Variations of the pyrolysis product ratios depending on the size were examined.

Poster Presentation : **ANAL.P-195**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Ionization behaviors of amino nitrotoluene in atmospheric pressure chemical ionization

He-Ryun Choi, Sung-Seen Choi*

Department of Chemistry, Sejong University, Korea

Amino nitrotoluenes (ANTs) are found as a naturally decomposing derivatives of 2,4,6-trinitrotoluene (TNT) in a wide range of land and groundwater. In aerobic conditions, the promising decomposition product from TNT to ANT is 2-amino-4-nitrotoluene (2-A-4-NT). ANT detection can be an indicator to determine the presence of TNT in the area, and analysis of ANT is necessary because it adversely affects human health and the environment. In general, ANTs have been analyzed using high-performance liquid chromatography (HPLC) equipped with a UV detector. ANT isomers such as 2-A-4-NT, 2-A-5-NT, and 2-A-6-NT could be distinguished by gas chromatography/mass spectrometry (GC/MS) analysis. We analyzed six ANT isomers of 2-A-6-NT, 2-A-5-NT, 2-A-4-NT, 2-A-3-NT, 4-A-3-NT, and 4-A-2-NT using direct atmospheric pressure chemical ionization-mass spectrometry (APCI-MS). In this study, kinds and abundances of the product anions and cations of the six ANTs ionized by APCI were examined. Some ANTs could be distinguished among them by comparison of the ion abundance ratios. The ionization mechanisms and ionization efficiencies of the ANT isomers were discussed using the analysis results and the structure optimization calculations.

Poster Presentation : **ANAL.P-196**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

SERS-based serodiagnosis of acute febrile diseases using nanopopcorn microarray platforms

Kihyun Kim, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

It is essential to develop sensitive and accurate diagnosistic tool for acute febrile diseases because the current gold standard method called immunofluorescent assay (IFA) cannot give accurate and objective readout. To resolve this problem, we developed a surface-enhanced Raman scattering (SERS)-based immunoassay platform for the diagnosis of scrub typhus and murine typhus, which are the most common acute febrile diseases in South Korea. A microarray device, composed of multiple gold nanopopcorn substrates capable of detecting disease-specific biomarkers, was used as a multiplex SERS-based assay platform. We analyzed Raman signals from different titers of Orientia tsutsugamushi and Rickettsia typhi specific human IgG/IgM antibodies, which are biomarkers of two typhus diseases, and the peak intensity was plotted against each titer concentration range to generate calibration curves. The LODs of titer concentrations for O. tsutsugamushi IgG/IgM and R. typhi IgG/ IgM are determined to be 20.4, 7.03, 16.8 and 12.5, respectively. These LOD values all meet the cut-off values (256, 16, 128, and 64) used for clinical diagnosis, unlike conventional ELISA method. These results show that our SERS-based assay platform can accurately diagnose two typhus diseases with high sensitivity.

Poster Presentation : **ANAL.P-197**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

SERS-LFA strip for rapid classification of Influenza A and SARS-CoV-2

Mengdan Lu, Jaebum Choo[1,*]

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

The spread of COVID-19 has caused enormous economic and social losses worldwide. In addition, there is a prediction that there may be a flu epidemic at the same time this fall. Since influenza and COVID-19 have similar symptoms such as fever, cough, sore throat, muscle aches, and diarrhea, it is essential to quickly determine whether a suspected patient is infected with COVID-19 or Influenza to prevent the spread of COVID-19 effectively. Although a rapid immunochromatic kit has been commercialized for this purpose, it has low diagnostic reliability due to the false-negative issue and low sensitivity. To solve this problem, we developed a highly sensitive SERS-based lateral flow assay (LFA) strip that can detect influenza virus (H1N1) and COVID-19 simultaneously with high accuracy. According to our assay results, the limits of detection (LoDs) for influenza a virus (H1N1) and SARS-CoV-2 were 57 HAU/mL and 4 PFU/mL, respectively. These values are approximately 500 times more sensitive than those measured from commercially available rapid LFA kits.

Poster Presentation : **ANAL.P-198**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

An NIR emissive two-photon absorbing ratiometric nitroreductase probe for studying hypoxia susceptibility of organ tissues

Sourav Sarkar, Kyo Han Ahn[1,*]

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

Hypoxia, a condition of oxygen deficiency in tissues, features various diseases including solid tumor, ischemia etc. Under hypoxia, several reductase enzymes including nitroreductase (which reduces nitro substrates) are elevated. Based on this fact, we have investigated an indirect way to assess the hypoxia susceptibility of different organ tissues (mouse lung, heart, spleen, kidney, and liver) by detecting nitroreductase present within. Among the organs, the kidney showed a notable susceptibility to hypoxia, which was due to the renal medulla, not due to the renal cortex, as observed by ratiometric fluorescence imaging with a probe. The probe features ratiometric signaling, NIR-emitting, two-photon absorbing, and pH-insensitive emission properties, offering a practical tool for studying the nitroreductase activity and, furthermore, hypoxia-associated biological processes.

Poster Presentation : **ANAL.P-199**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

SERS-PCR Assays of SARS-CoV-2 using Au nanoparticles-inserted Au nanodimple substrates

Yixuan Wu, Jaebum Choo[1,*]

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

The reverse transcription-polymerase chain reaction (RT-PCR) method has been adopted worldwide to dignose severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). Although this method has good sensitivity and specificity, there is clearly a need to develop a more rapid diagnostic technology, given the virus's rapid spread. However, the RT-PCR method takes a long time to diagnose SARS-CoV-2 because of the required thermocycling steps. Therefore, we developed a surface-enhanced Raman scattering (SERS)-PCR detection method using an AuNP-inserted Au nanodimple substrate (AuNDS) to shorten the diagnosis time by reducing the number of thermocycling steps needed to amplify the DNA. For the envelope protein (E) and RNA-dependent RNA polymerase (RdRp) genes of SARS-CoV-2, when the initial DNA concentration was 1.00 × 10^5 copies/μL, 25 RT-PCR thermocycles are required to reach a detectable threshold value, while 15 cycles are required for magnetic bead-based SERS-PCR. However, only 8 cycles are needed for the AuNDS-based SERS-PCR, and the corresponding detectable target DNA concentrations were 3.36 × 10^12, 3.28 × 10^9, and 2.56 × 10^7 copies/μL, respectively. Therefore, AuNDS-based SERS-PCR is seen as being a new molecular diagnostic platform that can shorten the time required for the thermocycling steps relative to the conventional RT-PCR.

Poster Presentation : **ANAL.P-200**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Rapid and sensitive detection of SARS-CoV-2 using SERS-based microdroplet sensor

Sohyun Park, Jaebum Choo[*]

Department of Chemistry, Chung-Ang University, Korea

The coronavirus disease 2019 (COVID-19) has been labeled an ongoing pandemic by the World Health Organization (WHO). Real-time quantitative polymerase chain reaction (RT-qPCR) has been considered a gold standard for the quantitative evaluation of a target gene. However, it still suffers from the problem of a long detection time. Commercially available lateral flow assay kits can be taken within 30 min, but it has low sensitivity and poor accuracy problems. To address these issues, we developed a surface-enhanced Raman scattering (SERS)-based immunosensing platform for the rapid and sensitive detection of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). In this work, SERS nanoprobes, which are anti-SARS-CoV-2 nucleoprotein antibody-conjugated gold nanoparticles, and magnetic beads have been used to detect SARS-CoV-2 nucleoprotein. The Raman signals of SERS nanoprobes for magnetic immunocomplexes were measured under flowing conditions inside a microdroplet channel. Total analysis time from droplet generation to SERS detection takes less than 10 minutes because all experimental conditions were automatically controlled inside the exquisitely designed microfluidic channel. This novel SERS-based immunosensing platform using a microdroplet channel is expected to be a powerful analytical tool to detect SARS-CoV-2.

Poster Presentation : **ANAL.P-201**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Structural Characterization of Non-human Glycan Antigens in a Xenograft Model using Nano PGC LC/MS/MS and Exoglycosidase Digestion

Ji Eun Park, Dongtan Yin, Hyun Joo An*

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

Xenotransplantation is a potential solution to bridge the gap between donors and recipients, but differences in glycosylation between porcine and humans limit successful clinical trials. Recent studies have shown that galactose-α1,3-galactose(α-gal), NeuGc, and SDa act as epitopes triggering antibody-mediated rejection. Furthermore, it is essential to identify the glycan antigens on the surface because endothelial cells interact first with the recipient's immune component during the transplantation. Despite the emphasis on the importance of glycans in the immune system, studies on comprehensive characterization of glycosylation including the structure of xeno-glycan antigens in porcine are insufficient. Here, we performed overall glycan profiling and structural analysis of glycans with non-human moieties in porcine endothelial cells and serum using PGC LC/MS/MS and enzymatic digestion. We could identify various glycan isomers and heterogeneity characteristics by accurate masses, retention times, LC/MS/MS, and exoglycosidase digestion. We identified and quantified totally 93 N-glycans from serum as well as 80 N-glycans from cells. In particular, non-human glycans were present in an amount less than 10%. NeuGc-sialylated glycan portion in cell and serum is around 7% and 3%, respectively. Structures of numerous α-gal containing glycans were identified by tandem MS and enzymatic digestion using α-galactosidase, which cleaves gal α1-3 linkages at the terminal. Interestingly, a specific glycosylated form in which sialic acid attached to antennal N-acetyl glucosamine is identified only in cells, whereas the lactylation modification was confirmed in serum. Our data could be the reference for monitoring changes in glycan antigens in glycoengineering models for xenotransplantation.

This research was supported by a grant(21172MFDS192-1) from Ministry of Food and Drug Safety in 2021.

Poster Presentation : **ANAL.P-202**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Simultaneous Identification of Structural Analogs of Cyclic Imines in Marine Biotoxins Using LC-MRM/MS

Hee Young Jo, Sanggil Lee, Hyun Joo An[*]

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

Cyclic Imines (CIs), a family of marine biotoxins, have an imine functional group and spiro-linked ether moiety in common in their structure, and rapidly inhibit neuronal nicotinic acetylcholine receptors, leading to a potent neurotoxic effect. These CIs are produced by microalgae and can accumulate in the marine life food chain, thus exposing consumers to potential risks. However, due to the very low concentration of CI and high levels of analogues, safety management and analysis regulations have not yet been established. Therefore, it is necessary to preemptively manage regulatory and confirmatory method to prevent potential risk posed by CIs. Here, we have developed structure-based simultaneous analysis method for qualification and quantification of CIs using liquid chromatography/mass spectrometry (LC/MS) which is a powerful technique to separate and analyze complex mixture due to its high sensitivity and selectivity. Mixtures of CIs such as GYM-A, 13-desMe SPX C, 13,19-didesMe SPX C, 20-Me SPX G, PnTX-E, F, G were separated according to hydrophobicity on C18 column and profiled by accurate molecular weight. We identified structure-based the fragment pattern by CI types. And tandem MS (MS/MS) was performed while adjusting CID energy to generate an optimal fragment pattern. For instance, product ions commonly found in pinnatoxin (m/z: 164, 177, 204, 220, 230) can be used like fingerprint recognition for CI identification and specific product ions can be used to identify analogues of CI subtype. We also measured the limits of detection (LOD, 2ppt) and quantification (LOQ, 5ppt) with high reproducibility using LC-MRM MS. Ultimately, we will analyze and simultaneously monitor CIs around the Korean Peninsula using newly developed analytical platform.This research was supported by a grant (20163MFDS641) from Ministry of Food and Drug Safety in 2021.

Poster Presentation : **ANAL.P-203**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Simple fluorescence detection of spermine based on paper-based analytical device

Nguyen ngoc Nghia

Department of Materials Convergence and System Engineering, Changwon National University, Korea

The fluorescence (FL) quenching of the ciprofloxacin (CP)-Tb^{3+} complex, which emits a bright green emission, was used to develop a simple spermine detection method. Because spermine competes with Tb^{3+} ions for interaction with CP due to its positive charge, the coordination link between CP and Tb^{3+} is weakened. The probe has a low limit of detection of 0.17 M. Moreover, a paper strip test (PST) with the support of a smartphone and an Arduino device was designed. The results indicate the applicability and feasibility of the probe for spermine detection in real samples.

Poster Presentation : **ANAL.P-204**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fast and visual folic acid detection using paper-based analytical devices

DaeHyun Kwon

Department of Materials Convergence and System Engineering, Changwon National University, Korea

A paper-based analytical device (PADs) was developed for the colorimetric detection of folic acid (FA). The sensor was prepared by using rhodamine B derivative-Cu^{2+} (RhB-Cu^{2+}) as a color indicator. The color intensity of RhB-Cu^{2+} was enhanced significantly after adding analyte. It can be explained by the improvement of electron transfer from RhB-Cu^{2+} to FA. Moreover, a smartphone was applied to take images from PADs, then analyze color intensity via RGB parameters. This device can provide a simple on-site detection platform.

Poster Presentation : **ANAL.P-205**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Paper-based analytical devices for quercetin detection

Sonexai Phommachith

Department of Materials Convergence and System Engineering, Changwon National University, Laos

To determine quercetin, a paper-based analytical method was developed. Quercetin quantitative analysis based on the measurement of fluorescence emission between quercetin and Y^{3+} with a detection limit of 27 nM. To convert fluorescence emission to bias signals, a home-made reader was built by connecting an Arduino platform to a photodiode. Furthermore, a smartphone was utilized to determine hue value from paper strip fluorescence emission. This approach could be used to detect quercetin in real samples on-site.

Poster Presentation : **ANAL.P-206**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A smart approach for selective rutin detection utilizing bovine serum albumin

Le thi cam Huong

Department of Chemistry, Changwon National University, Vietnam

As a widespread kind of flavonoids, rutin and quercetin are present in fresh fruits, vegetables, and certain food supplements. Because of their wide variety of biological functions, low cost, and considerably high safety margins, bioflavonoids have found application in the healthcare system. Rutin and its aglycone quercetin have similar chemical structures and characteristics as a sort of bioactive flavonoid glycoside. It is still possible to predict rutin in the presence of quercetin in a precise and effective manner. In this study, a simple UV-vis method was used to investigate the effect of BSA and some amino acids in phosphate buffer solution (PBS) on rutin and quercetin absorbance. The results show that the quercetin was effectively masked by the BSA.

Poster Presentation : **ANAL.P-207**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Improve SERS using silver on chitosan nano-wrinkles substrate

Pham khanh Linh

Department of Chemistry, Changwon National University, Vietnam

Chemical and electromagnetic mechanisms are commonly known to induce the Surface-enhanced Raman spectroscopy (SERS) effect. The electromagnetic impact from the stimulation of localized surface plasmons (LSPs) near a nanoplasmonic surface augmentation is the subject of this work. To tailor the size and form of the silver nanoparticles, an inkjet microreactor was employed for deposition Ag on chitosan nano-wrinkles substrate. Silver nanoparticles were synthesized directly in the head nozzles of the inkjet printer via the reduction of silver nitrate ($AgNO_3$) by ascorbic acid. Furthermore, to obtain a reproducible and sensitive paper-based SERS substrate, the office paper was decorated with chitosan, which permitted the formation of randomly oriented nano-wrinkles on the surface, thereby enabling the formation of silver nanoparticles with good hotspots. The prepared paper-based SERS substrate demonstrated exceptional sensitivity, spot-to-spot, and batch-to-batch reproducibility for on-site detection of Rhodamine 6G using a portable Raman spectrometer. The limit of detection was calculated to be 10.7 pM. Remarkably, our paper-based SERS substrate has a superb enhancement factor (~ 7.4×10^8). The prepared SERS substrate is a promising candidate for point-of-care test applications.

Poster Presentation : **ANAL.P-208**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mineralization of Indigo Carmine Using $ZnBi_2O_4$-Bi_2S_3 Composites in Visible light

TaeJun Ju

Department of Materials Convergence and System Engineering, Changwon National University, Korea

Novel highly visible-light active $ZnBi_2O_4$-Bi_2S_3 photocatalysts have been synthesized by a simple two-step co-precipitation and hydrothermal method. The efficiency of the prepared $ZnBi_2O_4$-Bi_2S_3 composites was evaluated for the degradation of Indigo carmine in aqueous solutions under visible light irradiation. The photocatalytic activities of the prepared $ZnBi_2O_4$-Bi_2S_3 composites was higher than that of pristine $ZnBi_2O_4$. This enhancement could be attributed to synergetic effects, charge transfer between $ZnBi_2O_4$ and Bi_2S_3, as well as the separation efficiency of the photogenerated electrons and holes. These results demonstrate the feasibility of utilizing $ZnBi_2O_4$-Bi_2S_3 as potential heterogeneous photocatalysts for environmental remediation.

Poster Presentation : **ANAL.P-209**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis and characterization of $LiFeBO_{3-x}F_{2x}/C$ nanocomposite as cathode material for Li-ion batteries

Yujin Son, Youngil Lee*

Department of Chemistry, University of Ulsan, Korea

Lithium iron borate ($LiFeBO_3$, LFeB) is considered as a promising cathode material for lithium-ion batteries (LIBs) because of its high theoretical discharge capacity of 220 mAh g^{-1}. However, LFeB cathode is limited to use in commercial LIBs by its low electrical conductivity resulting in low electrochemical performances. Fluorine substitution at the oxygen sites of LFeB to improve its low conductivity has been conducted with phase transition from monoclinic to vonsenite, in previous study. After the first charge/discharge cycle, however, the discharge capacity is significantly reduced. To overcome this problem, we have studied to improve the stability of its structure by carbon coating at the surface of F-doped $LiFeBO_3$(LFeBF) with maintaining high discharge capacity. The carbon-coated LFeBF (LFeBF/C) have been successfully synthesized by solid-state reaction method and characterized by X-ray diffractometry (XRD), SEM, TEM, and ^{7}Li MAS NMR spectroscopy. The electrochemical properties of LFeBF/C have been measured by using Galvano static charge/discharge test with the potential range of 1.0 - 4.5 V.

Poster Presentation : **ANAL.P-210**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis and characterization of iodine-doped $LiFeBO_3$ as cathode for lithium-ion battery

Yujin Jeong, Youngil Lee[*]

Department of Chemistry, University of Ulsan, Korea

Among the types of cathode material for lithium-ion batteries, polyanionic compounds have higher thermal stability and better safety properties due to the strong covalent bond of oxygen atoms, which make them more suitable for large-scale applications of lithium-ion battery. Among iron-based polyanion compounds, LFeB ($LiFeBO_3$) is a promising cathode material because it has the lowest weight framework and provides a high theoretical capacity of 220 mAh/g. Therefore, there are various studies on anion-doping as a method to improve the poor electrical conductivity of LFeB. So herein, doping of iodine, a relatively less study in cathode materials, has been conducted. For iodine-doped LFeBI ($LiFeBO_{3-x}I_{2x}$), it is important to set an appropriate synthesis temperature because of the rapid sublimation of iodine. XRD measurement has been performed to confirm the phase change of LFeBI depending on doping ratio synthesized by solid-state reaction, and electrochemical performance evaluated to confirm the improvement of electrical conductivity.

Poster Presentation : **ANAL.P-211**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Study on the Effect of Ammonium ions on Yb/Lu Separation Efficiency

Aran Kim, Kang Hyuk Choi*

Radioisotope Research Division, Korea Atomic Energy Research Institute, Korea

The no-carrier added (nca) lutetium-177 (^{177}Lu, $t_{1/2}$ = 6.7 d) are a promising therapeutic radionuclide in nuclear medicine because it has high specific radioactivity and high radionuclide purity without long-lived radioactive impurity. The nca ^{177}Lu can be produced via the ^{176}Yb(n,γ)^{177}Yb → ^{177}Lu reaction, where the process of separating it from a macroscopic amount of Yb target is important. Ion exchange chromatography is generally used to separate two adjacent nuclides Yb and Lu, with α-HIBA (α-hydroxyisobutyric acid) as complexing agent and NH_4^+ (ammonium hydroxide) as separating ion. Numerous papers evaluating the separation efficiency have studied the effect of the concentration of the eluent, but few papers have evaluated the separation efficiency using separating ion other than normal NH_4^+ ion. Thus, in this study, the separation efficiency of stable isotopes Yb and Lu was evaluated by using different ammonium ions, including primary, secondary and tertiary ammonium ions, replacing NH_4^+ ion. Separation experiments were carried out using α-HIBA with pH adjusted using ammonium hydroxide, methylamine, ethylamine, diethylamine, pyridine, ethanolamine and ethylenediamine, respectively. Since the column retention time and elution time increase as the amine order increases, it is important to select an appropriate type of ammonium ion for effective and selective separation of Yb and Lu.

Poster Presentation : **ANAL.P-212**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis of $LiFe_{1-x}Mn_xBO_{2.7}F_{0.6}$ as a cathode material for Li-ion battery

Daeun Han, Youngil Lee*

Department of Chemistry, University of Ulsan, Korea

Among the cathode materials of lithium-ion batteries, borate-based materials have been studied a lot so far due to their high theoretical capacity (220 mAh g^{-1}). One of these borate-based materials, $LiFeBO_3$ has good stability, low open-circuit voltage (OCV), and good reversible capacity. In a previous study, we have shown that the discharge capacity of $LiFeBO_{2.7}F_{0.6}$ has been improved by doping fluorine into $LiFeBO_3$. However, structural instability has been observed. Therefore, in this study, manganese is added to the metal site of $LiFeBO_{2.7}F_{0.6}$ to acquire its structural stability. $LiFe_{1-x}Mn_xBO_{2.7}F_{0.6}$ (x = 0, 0.25, 0.5, 0.75 and 1.0) have been synthesized by solid-state method and characterized their structure by ^{7}Li MAS NMR and X-ray diffraction (XRD). The stability of the structure has also been verified by measuring the electrochemical performances with the Galvano static charge-discharge test.

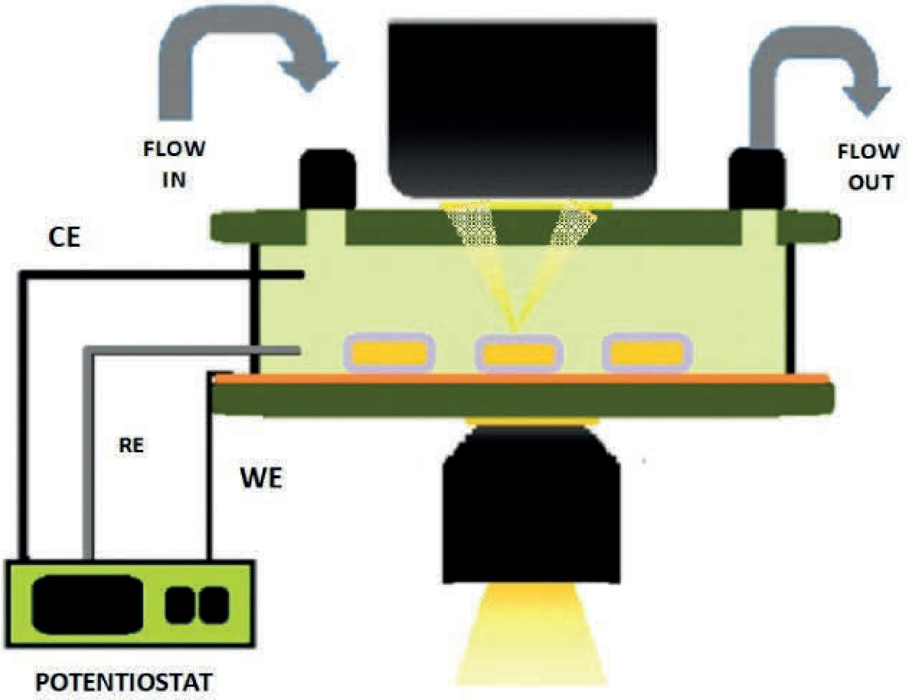
Poster Presentation : **ANAL.P-213**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Characterizing Mercury Amalgamation on Single Mesoporous Silica Coated Gold Nanorods Using Spectroelectrochemistry

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

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

Direct observation of chemical reactions in metallic nanoparticles is of great importance to have a deeper understanding of these processes for their uses in nanoparticle-based sensing and catalytic applications. Recently, scattering-based dark-field (DF) microscopy has been incorporated into electrochemical cells for enabling optical investigation of electrochemical processes on nanoparticle surface (Figure 1). In this spectroelectrochemical approach, electrodes constituted by low-density nanoparticles deposited on ITO substrates were used to inject electrons into nanoparticles whose optical response was then monitored by DF microscopy. In the present study, we used spectroelectrochemistry (electrochemistry + DF microscopy and spectroscopy) to characterize mercury amalgamation on gold nanorods coated with mesoporous silica shell (AuNRs@mSiO$_2$O) at the single particle level. Mercury (Hg^{2+}) was electrochemically reduced at AuNR electrodes, and the consequent optical changes resulting from deposition of mercury were monitored by scattering-based DF microscopy. Mesoporous silica shell allowed for approaching of mercury on the AuNR surface. Single AuNRs@mSiO$_2$O showed longitudinal surface plasmon resonance (LSPR) blue-shifts as well as a linewidth broadening in their scattering spectra, caused by the reduction (or amalgamation reaction) of mercury on the Au nanoparticle surface. Furthermore, reduction peaks were observed at potentials which were attributed to Hg^{2+} reduction under linear sweep voltammetry.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Poster Presentation : **ANAL.P-214**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis and characterization studies of Mn and Co composite as a cathode material for lithium secondary batteries

Hyeseung Kwon, Youngil Lee[1,*]

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

$LiMBO_3$ (M=Mn, Fe, or Co), a polyanionic lithium metal borate as a cathode material for lithium secondary batteries, is actively being studied because of its light weight, structural stability, and high theoretical capacity (220 $mAhg^{-1}$). Among borate-based polyanionic materials, $LiMnBO_3$ has high operating potential, $LiCoBO_3$ has high operating voltage and high theoretical (215 $mAhg^{-1}$). Herein, monoclinic $LiMn_{1-x}Co_xBO_3$ (x = 0, 0.25, 0.5, 0.75, and 1.0) cathode materials have been synthesized by solid-state reaction method. X-ray diffraction (XRD) and solid-state ^7Li MAS NMR spectroscopy have been measured to characterize the crystal structure. Galvano electrostatic charge/discharge tests for prepared samples have been also studied to identify oxidation/reduction potential and operating voltage. Quantitative analysis of the chemical composition of the material has been also performed by laser-induced destructive spectroscopy (LIBS) and inductively coupled plasma-optical emission spectroscopy (ICP-OES).

Poster Presentation : **ANAL.P-215**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Capture of microplastics and subsequent quantitative analysis using Raman spectroscopy

Yunjung Kim, Hoeil Chung[*]

Department of Chemistry, Hanyang University, Korea

Microplastics (MPs) are known around the world as materials that destroying ecosystems. A typical method of analyzing MPs in water is the separation of MPs using diverse filters and measurement of the filtered MPs using diverse spectroscopic tools such as IR and Raman spectroscopy. Alternatively, for on-line detection, perfluorohexane (PFH, C_6F_{14}) was used as an MPs-capturing medium in this study. As known, PFH is highly hydrophobic, thereby potentially attracting MPs. When water samples containing polyethylene (PE) particles was flowed through a PFH droplet, the PE particles were captured by the PFH droplet. Then, a wide area illumination (WAI) scheme providing a laser diameter of 6 mm was used to collect Raman spectra of captured PEs. In the collected spectra, the intensity ratio of PE and PFH peaks clearly increased as the amount of PE particles increased. Meanwhile, the particle size of MPs considerably varies and the corresponding Raman intensity also differ depending on the particle size. Therefore, for reliable quantitative analysis, a Raman measurement cell able to overcome the particle size-inducing spectral variation has been searched and its potential will be discussed.

Poster Presentation : **ANAL.P-216**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Metabolite Profiling of Korean Chestnut (Castanea crenata S. et Z.) fruits using UPLC-MS Analyses

Min-sun Kim*, Mi So Nam

Food Analysis Research Center, Korea Food Research Institute, Korea

Chestnuts are extensively grown a major starch crop plants. In this study, we determined the difference in the metabolic composition of Korean chestnuts (Daebo, Okkwang, Ipyeong) using ultra-performance liquid chromatography (UPLC)-quadrupole time-of-flight (QTOF) mass spectrometry. The principal component analysis model generated from the mass spectrometry data showed significant separation among groups. The characterization of metabolites related to Chestnuts species was confirmed by high resolution MS analysis using QTOF, with the calculation of the corresponding molecular formulae. The Daebo was rich in antioxidant compounds such as ascorbic acid, catechin, and phloretin. The discriminant metabolites, especially, Cytidine, Glutamine, and Proline were higher in Daebo. The Okkwang had abundant p-coumaric acid, tryptophan, and tyrisine. Syringic acid O-glucoside, the class of organic compounds known as hydrolyzable tannins, was abundant in Ipyeong. These metabolite profiling to identify primary and secondary metabolites are potentially helpful for Chestnuts selection and improvement.

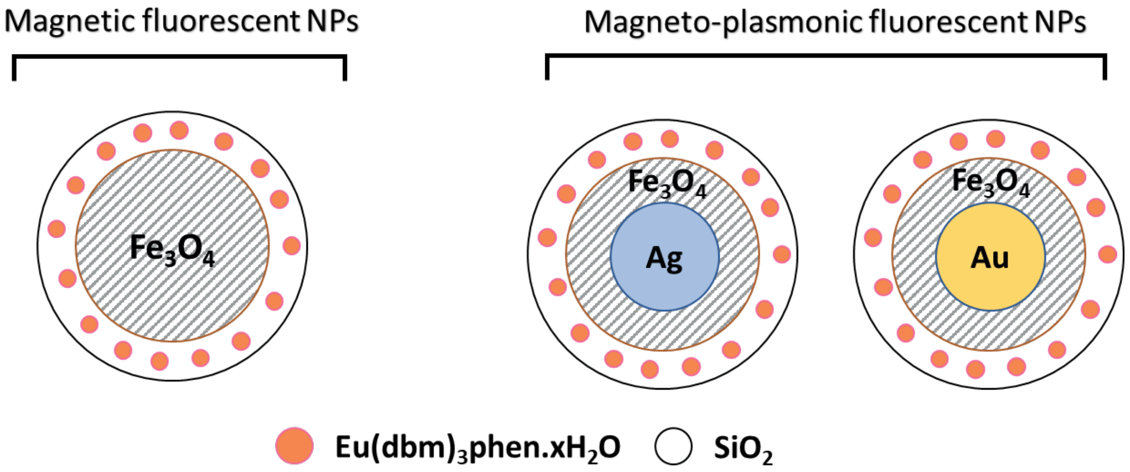
Poster Presentation : **ANAL.P-217**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Rare earth doped Magnetoplasmonic nanoparticles for the detection of heavy metal ions in water

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

Department of Chemistry, Chungnam National University, Korea

Compared to fluorescent organic dyes or quantum dots, rare earth phosphors show superior luminescent lifetime, minimal photo-bleaching and enhanced biocompatibility. Moreover, the unique properties of the base nanoparticles such as magnetism or photonic effects could be utilized to enhance or modify the emission characteristics of the fluorophores. In this study, multifunctional RENPs based on magnetoplasmonic core-shell nanoparticles having both magnetic, plasmonic and photoluminescence properties were fabricated. The base magnetoplasmonic nanoparticles were synthesized using facile one-pot solvothermal methods, and doping of fluorescent rare-earth chelates using a modified sol-gel method were performed. The synthesized Eu-RENPs with Ag@Fe3O4 MagPlas NP cores shown enhanced photoluminescent emission intensities of over 50% compared to non-plasmonic MNPs doped systems, achievable by the local enhancement effect of the plasmonic core. The absolute quantum yield of the synthesized product reached as high as 30% by adjusting the Eu chelates doping ratio. Moreover, the synthesized MagPlas Eu-RENPs were utilized as a selective sensing probe for the determination of copper(II) ions in water. It is discovered that the energy transfer process to the localized transition metal ions, especially copper(II), resulted in the selective quenching of the fluorophore, which were highly proportional to the Cu2+ concentration in the range of (0.05 to 5 mg/L). The limit of detection and quantitation of this method fulfilled the requirements for determination of copper concentration in drinking water. Overall, magnetoplasmonic RENP probes are highly prominent for environmental monitoring, sensing and imaging applications.



Magnetic fluorescent NPs
Magneto-plasmonic fluorescent NPs
Fe_3O_4
Fe_3O_4
Ag
Fe_3O_4
Au
$Eu(dbm)_3phen.xH_2O$
SiO_2

Poster Presentation : **ANAL.P-218**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Adsorption of Organic Dyes on Zeolitic Imidazolate Framework-8 Coated with Silica(ZIF-8@SiO_2)

Jian Choi, Seyeon Yang[1], Seog Woo Rhee[1,*]

chemistry, Kongju National University, Korea
[1]Chemistry, Kongju National University, Korea

In this study, the synthesis of silica-coated Zeolitic Imidazolate Framework-8(ZIF-8@SiO_2) and the adsorption behavior of organic dyes on the ZIF-8@SiO_2 were investigated. ZIF-8 was synthesized in a methanol media and its surface was coated with SiO_2 by hydrolysis of tetraethyl orthosilicate in a ethanol media. The physicochemical properties of the solid materials were investigated using SEM, EDS, FT-IR, XRPD, TGA, BET, and elemental analysis. The removal of organic dyes(methyl orange, phenol red, trypan blue) from aqueous solutions by adsorption onto ZIF-8@SiO_2 was investigated using batch experiments, and the adsorption capacity of organic dyes was evaluated based on the adsorption isotherms. The results of this study provided the potential of ZIF-8@SiO_2 as an organic dye adsorbent.

Poster Presentation : **ANAL.P-219**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Recognition of bile components in bile using Au nanodendrite substrates modified with various alkanethiols as a tool for Raman spectroscopic identification of gall bladder cancer

Thu Thuy Bui, Hoeil Chung*

Department of Chemistry, Hanyang University, Korea

In gall bladder (GB), bile juice is stored and could be a valuable specimen for relevant GB disease diagnosis, since its composition would vary depends on pathological conditions of GB patients. Therefore, this study intends to investigate the potential for Raman spectroscopic discrimination of GB polyp and GB cancer using the aqueous phase samples extracted from 32 raw bile juice samples. Initially, an alkanethiol was conjugated to the surface of a SERS substrate (Au nanodendrite on Ni foil (AuND@NiF)) to generate SERS signal and attract bile components via mutual interaction. For more effective and thorough recognition of bile components, 4 independent substrates covered with 4 different alkanethiols with various functional groups ($SH(CH_2)_2CH_3$, $SH(CH_2)_2NH_2$, $SH(CH_2)_2COOH$, and $SH(CH_2)_2OH$) were prepared. When aqueous phase bile samples were measured using each substrate, varied SERS peaks in each case were mutually characteristics. When the principal component (PC) scores of spectra obtained using the $SH(CH_2)_2CH_3$- and $SH(CH_2)_2OH$-covered substrates were combined, the *k*-Nearest Neighbor based discrimination accuracy was 100%, superior to those (90.6-96.9%) using individual substrates. The use of complementary bile component-induced spectral information of these substrates was attributed to the superior discrimination performance.**Keywords:** Bile; Gall bladder cancer; Au nanodendrite; SERS

Poster Presentation : **ANAL.P-220**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Optically tunable plasmonic chiral superstructure

Siyeong Hwang, Juyong Gwak[1], Jaebeom Lee[2,*]

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

2D metasurfaces have engaged enormous academic attention from their properties of manipulating polarized light and relatively facile fabrication. A new facile fabrication method for 2D chiral metasurface using magnetic field-induced nanoarray was proposed herein to make amend of current 2D metasurfaces and to develop dynamic in-situ tenability. The tunability of a chiroptical response was certified through adjustments of the curvature applied to the substrate. The application of the curvature induced a skew angle which is an angle between pattern direction and curvature, and it broke the symmetry of the structure which resulted in chirality. When the skew angle got closer to ±45°, a circular dichroism spectrum intensity got bigger which means the chiral response was enhanced. This extremely facile fabrication approach to magnetic self-assembly nanoarray inspires possibilities of mass production and a wide-range detection.

Poster Presentation : **ANAL.P-221**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Analysis of Body Odor using GO;PANI/ZNRs/ZIF-8 adsorbent followed by GC/MS

Sehyun Kim, Sunyoung Bae[1,*]

Chemistry, Seoul Women's University, Korea
[1]*Department of Chemistry, Seoul Women's University, Korea*

Human body odor offers important information about skin aging, sexual activities, and health status. Various human body odor comes from different interactions between eccrine, sebaceous, apocrine gland, and skin bacteria. trans-2-Nonenal, benzothiazole, hexyl salicylate, α-hexyl cinnamaldehyde, and isopropyl palmitate that considered as key indicators of skin aging were selected as target compounds. Solid phase microextraction (SPME) is commonly used to analyze body odor. However, SPME can be easily damaged and uncomfortable to collects body odor directly. To overcome this disadvantage, in-needle microextraction (INME) using graphene oxide; polyaniline/zinc nanorods/zeolitic imidazolate framework-8 (GO;PANI/ZNRs/ZIF-8) adsorbent followed by gas chromatography/mass spectrometry (GC/MS) was developed. The adsorbent could adsorb both nonpolar and polar volatile organic compounds because hydrophobic ZIF-8 and hydrophilic ZNRs were coexisted. By using the developed adsorbent, human body odor was extracted efficiently and determined by GC/MS. The amount of reactants involved in the fabrication of adsorbent and analysis condition were optimized using design of the experiment (DOE) method. The body odor of Korean women at the age of 20s ~ 70s were analyzed using the developed analysis method. As a result, it was confirmed that there was a difference in the amount of body odor generated by age.

Poster Presentation : **ANAL.P-222**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Identification of Secondary Organosiloxane Aerosol (SOSA) Using Aerosol Mass Spectrometry

Hwajin Kim

Environmental Health, Seoul National University, Korea

Volatile methyl siloxanes (VMS) are high-production chemicals emitted from many personal care products. Evidence from laboratory and ambient studies indicates that oxidized VMS products are present in particle phase and contribute to the formation of secondary organosiloxane aerosol (SOSA) . SOSA has most commonly been identified based on filter sampling and post-analysis. However, due to the low time resolution and time-consuming nature of offline methods, along with the sampling/storage artifacts, these methods are not ideal.In this work, we generated SOSA from oxidation of decamethylcyclopentasiloxane (D5, $C_{10}H_{30}O_5Si_5$) using an Aerodyne potential aerosol mass oxidation flow reactor (PAM OFR). The chemical composition of SOSA was characterized by high-resolution time of flight aerosol mass spectrometer (HR-ToF-AMS). In particular, we operated the instrument at an m/z range of up to ~1080 and for the first time observed a series of high-molecular ions of SOSA in the AMS mass spectra.Although the ability of AMS to characterize molecular composition is limited, the SOSA ions ($C_wH_xO_ySi_z$) can be identified by AMS. We also found the mass spectra from SOSA contained distinct groups of monomers, dimers and trimers, which reveals that the particles are composed mainly of products of D5 oxidation. The technique demonstrated here may offer new insights into characterizing SOSA related species and further can be used to identify the SOSA trace from ambient measurements both from indoor and outdoor.

Poster Presentation : **ANAL.P-223**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fabrication of highly acid-resistant coating material using keratin

Jungwoo Suh, Kwanwoo Shin[1,*], Soo Ryeon Ryu

Institute of Biological Interfaces, Sogang University, Korea
[1]*Department of Chemistry, Sogang University, Korea*

Keratin is a type of protein that makes up hair, skin, and nails. Keratin is also known as a protective protein that mechanically protects body tissues. Therefore, it has been used as a biopolymeric material in various fields by using its excellent biocompatibility and excellent mechanical property. In addition, it is known that keratin has excellent chemical properties and, in particular, has a high acid-resistant property. In this study, focusing on the acid-resistant property of keratin, a stable keratin thin film was fabricated on the surface as a highly acid-resistant coating material. To improve the performance of the film, formic acid and glutaraldehyde were introduced to make a cross-linked insoluble thin film. The acid-resistant property was confirmed by treating the formed film with a pH 1 HCl solution and a saturated HCl solution (pH 0.1), respectively, and structural changes were analyzed with FT-IR and electron microscope.

Poster Presentation : **ANAL.P-224**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Nanomechanical identification of the mutated EGFR signaling systems on the living lung cancer cells and their extracellular vesicles

Soohyun Park, Yoonhee Lee[*]

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

Epidermal growth factor receptor (EGFR) is the transmembrane glycoprotein inducing cell differentiation and proliferation. Receptors are located at the cell surface, where the binding of the ligand activates a tyrosine kinase in the intracellular region. The overexpressed and mutated EGFR enables tumor cells to become independent of external growth control cues and drives persistent survival signaling.1 The plasma membrane of cancer cells has significant changes in its structure and organization to support growth factor signaling. The signaling activity of the plasma membrane is influenced by its biophysical properties, including fluidity, charge, and local architecture. For example, the clustering of EGFR molecules into the lipid rafts indicates that these highly ordered and rigid nanodomains function as signaling platforms.2 Also, the altered growth factor signaling mediated by the mutated EGFR can determine the levels of major lipid classes, resulting in the change of the plasma membrane composition.3 However, how the altered EGFR signaling regulates the membrane elasticity and changes the lipid raft structure are not well understood. Here, we detect and quantitatively measure the nanomechanical properties of the EGFR clustered lipid rafts in the plasma membranes from the four types of living lung cancer cells and their extracellular vesicles using atomic force spectroscopy (AFM). We employ anti-EGFR antibody-attached AFM probe that binds to the single-molecule EGFR to locate the EGFRs on the surface. At the same time, the AFM probe measures the elasticity of the EGFR clustered lipid rafts by applying nanoindentations. This study can identify the biophysical relationship between genetic mutations in the growth factor signaling system and the reorganization of the plasma membrane composition.Reference1.Lin, C. C. et al. Theranostics 2020, 10, 10925-10939.2.Guéguinou, M. et al. Biochim. Biophys. Acta 2015, 1848, 2603-2620.3.Bi, J. et al. Cell Metab. 2019, 30, 525-538.e8.

Poster Presentation : **ANAL.P-225**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Formation of Wrinkling Patterns for Flexible Electrodes by Using Direct Printing

Yeeun Jo, SeungYeon Lee, Kwanwoo Shin*, Oh-Sun Kwon

Department of Chemistry, Sogang University, Korea

Forming a flexible electrode on an elastomer surface is useful in the field of wearable devices that require repeated bending and folding. A wrinkled electrode has received much attention as an effective flexible electrode. In most cases for wrinkled electrode patterns, however, pre-stretching or thermal expansion of the substrate is required. In this study, we confirmed that the wrinkled electrodes can be directly printed and formed by a direct printing method that does not require pre-processing or post-processing. We found that the wrinkle pattern was induced by the interaction between ozonated elastomer and the solvent of the ink. The printed wrinkle patterns, depending on the solvents, oxidation time, and printing speed of silver ink were monitored and compared. It was confirmed that the wrinkled patterns produced by our method maintained stable conductivity under mechanical bending stress and could be used for wiring of various flexible electronic devices.

Poster Presentation : **ANAL.P-226**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Formation of Two-Dimensional Au/MoO^3 Hybrid Nanostructures by Growth and Exfoliation

Jihoon Park, Youngsoo Kim*

Department of Chemistry, Yeungnam University, Korea

Two-dimensional nanomaterials separated from bulk have received many attention because of their unique properties. Differ from the bulk property, they exhibit high-conductivity, high-mechanical strength and unique optical properties, so they have vast applicability in the research and industrial field. Various method to prepare 2-dimensional materials have been studied using mechanical and electrical forces. These methods, which are classified as Top-down approaches, have weaknesses like hard to control the thickness of layers and generation of lots of defects on the surface. In this study, we synthesized Au/MoO_3 heterostructures by intercalation of Au ions and growth of Au nanoparticles, and exfoliation of MoO_3 layers sequentially. The hybrid Au/MoO_3 nanostructures prepared were characterized by UV-Vis spectrophotometer, TEM, and XRD. We hope the hybrid nanomaterials could be applicable for photocatalysts and electronic devices

Poster Presentation : **ANAL.P-227**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Magneto-Plasmonic Metasurface sensor for Circulating Tumor Cell Molecular Beacon at Terahertz regime

Young-Mi Kim, Jaebeom Lee[1,*]

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

Terahertz (THz) waves have great potential for wide applications in imaging, sensing, and other fields. However, due to the lack of strong response materials for efficient generation, and detection of THz waves, many researchers introduce metamaterials that afford the generation, polarization, sensing, and imaging in THz waves. Metamaterials, artificially designed by changing their unit cell. Herein, new THz metamaterials, Ag@Fe3O4 magneto-plasmonic (MagPlas) nanoparticles (NPs) are coated on the unit cell of the nickel-patterned metasurface. By magnetizing the metasurface, NPs can be assembled with the ferromagnetic properties of nickel on the surface. On the magnetized metasurface with MagPlas NPs, THz resonance with improved sensitivity of Circulating tumor cells (CTCs)-derived microRNAs (miRs) sensing. That biomarker, CTCs miRs, in blood and tissues have been fascinated as novel noninvasive biomarkers for monitoring tumor progression. Combination of metamaterials and MagPlas NPs was exploited to develop an ultrasensitive THz biosensor with high sensitivity. Using this platform, the biomolecule, CTCs miRs, can be combined with NPs, which shows the potential for development to the biosensor.

Poster Presentation : **ANAL.P-228**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

The effect of water and heavy water on fibrillation dynamics of intrinsically disordered proteins

MyungKook Son, Chae Ri Park, Sooyeon Chae, Dongjoon Im, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Amyloid proteins undergo self-assemblies to form insoluble fibrillar aggregates with a highly ordered □-sheets. These fibrils are associated with various human diseases, known as amyloidosis. To study amyloid-associated protein dynamics, various spectroscopic techniques such as Nuclear Magnetic resonance (NMR) spectroscopy, Infrared (IR) spectroscopy, etc. are utilized for the structural analysis. To avoid spectroscopic peak interferences such as H resonance frequency or O-H vibrational frequency in NMR and IR spectroscopy, deuterium oxide (D2O) is commonly used as a solvent for a deuteration of sample molecules. However, due to isotope effect of D2O, hydrogen bonding and hydrophobic effect are known to have stronger effect compared to H2O. Recently, we have found that D2O stabilize the folding structures of insulin, due to enhanced H-bonding and hydrophobic effect, inhibiting the fibrillation of insulin. In this research, we used α-synuclein and K18 to study the effect of reinforced hydrophobic effect on the intrinsically disordered protein (IDP) structures and protein stability-fibrillation. Small angle X-ray scattering (SAXS) and ion mobility mass spectrometry (IM-MS) were utilized for the study of solution phase and gas phase initial protein structures, and thioflavin-T (ThT) assay, circular dichroism (CD) and transmission electron microscopy (TEM) were utilized to compare the fibrillation kinetics in H2O and D2O.

Poster Presentation : **ANAL.P-229**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Plasmonic Au Nanoparticles Catalyzed Photodegradation of Lignin Derivatives

Jiwon Kang, Youngsoo Kim[1,*]

School of Chemistry and Biochemistry, Yeungnam University, Korea
[1]*Department of Chemistry, Yeungnam University, Korea*

Lignin is a major component of lignocellulosic biomass that is the most abundantly useable fuel on the earth. Natural lignin is a potential source to produce aromatic compounds as a petroleum alternatives. For this reason, researchers have been interested in the degradation of lignin compounds and have conducted various studies. Among the many methods for converting lignin, photocatalytic chemical transformation is a valuable work to obtain functionalized aromatic compounds that have been applicable to fine chemicals, biofuels, polymer industries, and pharmaceuticals. In this study, we carried out the conversion of β-O-4 lignin model compounds with plasmonic Au nanoparticles and visible light. We characterized the photodegradation organic substance with HPLC, NMR, IR, and MS.

Poster Presentation : **ANAL.P-230**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fabrication of Polymer-Au Hybrid Nanocomposite by Interaction of Gold Nanoparticles and Visible Light

Jeonghyeon Lee, Youngsoo Kim*

Department of Chemistry, Yeungnam University, Korea

High-performance polymeric materials can be applied in variety industrial fields such as chemistry, biochemistry, biology, and material science. Although there are many materials in high-performance polymer, we chose the polymeric nanocomposite that has great merit to use for liquid crystal, polarized film, thermal therapy, bio-imaging, and drug-delivery. It was synthesized by using the photothermal property of Au nanoparticles, resulting from the interaction with electromagnetic radiation. When Au nanoparticles absorb light, it can create both energetic charge carriers (i.e., hot electrons) and thermal energy through light-to-matter interaction. Those energetic particles can be acts as an initiation source to proceed polymerization at the surface of Au NPs. In this study, we pursued photo-polymerization of acrylic acid on Au NPs under visible light with control of irradiation intensity and excitation wavelength. The resultant was characterized by UV-Vis spectrophotometer, TEM, FT-IR, and so on. Consequently, we observed that poly(acrylic acid) was wrapped on the surface of Au NPs with a varying thickness depending on the experimental conditions.

Poster Presentation : **ANAL.P-231**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Comparing equilibrium structures of the Amyloid-β (1-42) dimers and assembly properties *in vitro*

Dongjoon Im, MyungKook Son, Chae Ri Park, Sooyeon Chae, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Senile plaque of Amyloid-β (1-42) is well-known pathological hallmark in Alzheimer's disease. High aggregation propensity is a major characteristic of Amyloid-β (1-42). In the previous study, we investigated equilibrium ensembles of Amyloid-β (1-42) on the basis of 19.2 μs replica exchange molecular dynamics simulations (400 ns per replica). From this simulation results, we confirmed that hydrophobic interaction plays a pivotal role in the self-assembly process of Amyloid-β (1-42) and contacts between side chains occur frequently in the specific domain. We also observed that substitution of the hydrophobic core residues into hydrophilic amino acid decelerates its fibrillation process. Herein, we obtained equilibrium ensembles of mutant peptide homo dimer and hetero dimer with wild type. To further investigation of inter-molecular states, we performed Markov State Model analysis. The free energy landscape of mutant peptide has multiple local minima whereas the wild type had only one global minimum state. Combined with mass spectrometry analysis, we can understand the underlying mechanisms in kinetical delay of the self-assembly process of Amyloid-β (1-42) with its point mutant.

Poster Presentation : **ANAL.P-232**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Sensing chiral analytes with chiral structure

Hwayoung Choi, Siyeong Hwang[1], Jaebeom Lee[2,*], Sejeong Park[3]

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

The method of separating and sensing monomer, oligomer, and polymer, which are enantiomeric molecules, is a very important issue in the pharmaceutical and biomedical fields. Circular dichroism spectroscopy can be used as a sensor of organic molecules but it has a technical limit of detection. Herein we introduce the magnetoplasmonic nanoparticle (MNP) to sensing chiral analytes. Helically aligned nano chains show remarkable circular dichroism and signal enhancement by plasmon resonance of Ag core. In our previous experiments, we analyzed chiral analysis in a liquid state. However, in liquid state, there is a problem with the fluidity of magnetic nanoparticles. So, we analyzed chiral materials in a fixed state. Two glass plates were used to analyze the chiral analysis using the chiral nematic structure. When the right or left circularly polarized light interacted with the chiral molecule, the particular spectrum of circularly irradiated light is observed compared with the same system without the chiral molecule. This result suggests that signal enhancer will be developed into a measurable, qualitative, and quantitative detector.

Poster Presentation : **ANAL.P-233**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Multifunctional Optical Probes in Dynamic Biological Environments Using Mesoporous Silica Shell Coated Single Gold Nanorods

Geun Wan Kim, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

Mesoporous silica coated gold nanorods (AuNRs@mSiO_2) are promising multifunctional orientation probes that can be employed in biological studies due to their anisotropic optical properties, enhanced stability, and excellent biocompatibility. In this paper, we characterized the optical properties of single AuNRs@mSiO_2 under dark-field (DF) microscopy and differential interference contrast (DIC) microscopy and demonstrated the application as orientation probes in a dynamic biological environment. First, we obtained the periodic DIC images and intensities of single AuNRs@mSiO_2 at their localized surface plasmon resonance (LSPR) wavelengths with high sensitivity. Furthermore, we successfully tracked the real-time rotational motions of the AuNRs@mSiO_2 on the live cell membranes with millisecond temporal resolution. this study will be beneficial for potential applications, as a multifunctional optical probe that can determine the orientation of probe and delivery appropriate drug to target cell.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **ANAL.P-234**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and characterization of hollow nanostructures

Hwayoung Choi, Jaebeom Lee[1,*]

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

Hollow core-shell nanostructure is a nanostructure composed of a void core instead of a solid core. Hollow nanosturucture has unique properties such as high surface-to-volume ratio and large pore volume, so researchers have been developed several synthetic routes.We synthesized hollow nanoparticles and hollow nanorods by galvanic replacement reaction and characterized these particles using UV-Vis spectroscopy, SEM, and zeta potential. These particles can be used for drug delivery, catalysis, and sensors using their porous properties, as well as for magentic assembly and magnetic hyperthermia treatment by using an external magnetic field due to the magnetic properties of the shell.

Poster Presentation : **ANAL.P-235**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A disposable capillary-driven electrodynamic microfluidic channel sensor for the separation detection of saccharides in whole blood sample

Mohammad Mozammal Hossain, Kyeong-Deok Seo, Yoon Bo Shim*

Department of Chemistry, Pusan National University, Korea

A disposable capillary-driven electrodynamic microfluidic channel sensor was fabricated with screen printed method for the separation detection of saccharides in a whole blood samples. The device was constructed with a separation channel and sensing parts on a single plastic substrate, where a hydrophilicity-controlled film lid was covered to form separation channel. Au-Mn dendrite was formed on conducting polymer (3',4'-diamino-2,2'; 5'2''-terthiophene (pDATT) as a sensor probe and demonstrated for the catalytic oxidation of saccharides. The flow of the dispensed liquid is driven by capillary forces without external energy input and electrodynamic force with AC field to precisely separate multitargets. Capillary flow rate in different hydrophilicity were experimentally monitored and compared using various lid plastics. The analytical parameters have been optimized affecting separation and detection performance in terms of AC frequency, AC amplitude, fluid flow rate, and detection potential. The calibration plots for the saccharides were found to be a wide linear range from 0.1 to 11.0 mM with the detection limits between 0.031 mM with LSV. Interference effects were also investigated, and the reliability of the proposed device was evaluated by the determination of saccharides and their concentration in real human blood samples.

Poster Presentation : **ANAL.P-236**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Colorimetric tensile Sensor from an array of plasmonic magnetic photo-crystal on a flexible substrate

Dajeong Hwang, Seonghwan Jung, Jaebeom Lee*

Department of Chemistry, Chungnam National University, Korea

The plasmonic effect is also used in color change devices using noble metal nanoparticles. These particles form a chain structure, form a plasmon coupling, and have a plasmon resonance on the surface. The reflectance of the surface changes by physical force, which is used for color sensors. Plasmonic noble metal particles form a plasmon coupling forming a chain structure and has plasmon resonance on the surface. The reflectance of the surface is changed by physical force, and this characteristic is used in color sensors. For example, Au noble metal colloidal nanoparticles can be seen using plasmon resonance characteristics to show a color change. Ag@MNPs a film sensor using nanoparticles can visually represent a physical change and apply it to various movements. In this paper, only physical reactions will show that the color changes without current and explain the principle. This will be able to achieve the purpose as a sensor by showing a definite change that differs from the saturation or brightness.Signals transmitted as electrical signals have many advantages, but the need for low power, flexible sensors for long time use is increasing. To solve this wearable device problem, this paper attempts to fabricate a low-power, flexible physical sensor using photonic crystals and to verify the results of various experiments.

Poster Presentation : **ANAL.P-237**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Investigation of TPT-VCR multidrug mechanisms in 3D spheroids human neuroblastoma cells

Sooyeon Chae, Chae Ri Park, MyungKook Son, Dongjoon Im, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Neuroblastoma is a common extracranial solid tumor in childhood, which begins when immature nerve cells grow out of control in the adrenal gland, abdomen, pelvis, chest, and neck. Multidrug regimen chemotherapy has been underway to optimize therapeutic outcomes, maximize treatment efficiency. The multidrug regimen with topotecan and vincristine was used for neuroblastoma patients. Topotecan (TPT) is an anti-tumor drug that forms a ternary complex into [topoisomerase I-DNA-TPT], preventing DNA replication. Vincristine (VCR) is also an anti-tumor drug, and its mechanism of action is interaction with tubulin to inhibit mitosis. Several clinical tests showed that the multidrug regimen with TPT and VCR have synergistic toxicity. However, the specific mechanism of this effect is still ambiguous due to challenges at mimicry of pharmacokinetics and the tumor microenvironment at the laboratory level. In this study, we aim to investigate TPT-VCR multidrug mechanisms and mimic pharmacokinetics and tumor microenvironment. 3D spheroid SK-N-SH neuroblastoma cells treated with TPT and VCR multidrug showed a synergistic effect compare to single-drug treatment. The tubulin polymerization data showed that the action of vincristine was reduced in multidrug treatment, which implies another pathway for a synergistic effect. For more detailed investigation, we plan to mimic pharmacokinetics and tumor microenvironment using A fluidic system.

Poster Presentation : **ANAL.P-238**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Development and validation of saliva collection and extraction method for metabolite profiling using UPLC-QTOF-MS

Miso Nam, Min-sun Kim*

Food Analysis Research Center, Korea Food Research Institute, Korea

Human saliva, with its advantages of easy and non-invasive collection, is increasingly being used for diagnosis, monitoring systemic disease status, and predicting disease progression. Saliva metabolomics has been relatively under-researched, compared to blood or urine, despite growing interest in recent years. In this study, saliva collection process and sample preparation method were developed and validated by metabolite profiling. Ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC-QTOF-MS) was used to identify metabolite changes depending on saliva collection and extraction method. A total of 50 metabolites, including amino acids, purine and pyrimidine derivatives, and organic acids, were identified in saliva samples. Comparing the saliva collection method using Salivettes cotton swab with direct tube collection method, it was confirmed that the method of collecting directly in a tube showed better sensitivity of most metabolites intensities. After sample collection, metabolite changes in saliva sample stored at RT and 4°C were evident, but most metabolites were unchanged at -20°C except for adenosine, guanosine, and inosine during short-term storage. A liquid-liquid extraction using acetonitrile compared to methanol for sample preparation showed highly sensitive detection of some metabolites. Our study suggests considerations for metabolite profiling using saliva samples.

Poster Presentation : **ANAL.P-239**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Signal processing for a real-time handheld biological monitoring system using an UV LED as a light source

Young-Su Jeong

Chem-Bio Technology Center, Agency for Defense Development, Korea

Real-time monitoring and warning technology of the atmosphere has gained importance in military and civilian biodefense. As the first stage of biodefense process, a trigger is a low power, compact, fast response sensor capable of reporting out a tentative warning. Previously we developed a small real-time ambient bioparticle monitoring system using laser induced fluorescence technology. Within it, we implement a simple and robust signal processing scheme for conversion from analog voltage into information of particle flow, suitable for portable triggers. An adaptive window to characterize the particle sizes increases the dynamic range of the particle counts as well as the size information of them. We confirmed the performance of the bioaerosol monitoring system by comparing it with APS.

Poster Presentation : **ANAL.P-240**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Recent research trends in direct identification of microorganisms by MALDI-TOF MS

Young-Su Jeong

Chem-Bio Technology Center, Agency for Defense Development, Korea

Matrix-assisted laser desorption time of flight mass spectrometry (MALDI-TOF MS) based identification also has significantly lower operational cost, which are the minimum requirements for substrates and reagents for option extraction. Based on these advantages, MALDI-TOF MS was used in wide applications such as clinical, food, military, and ecology research fields. But, the MALDI-TOF MS method has many challenges including that the MALDI-TOF MS identification is limited by the reference spectrum. This presentation briefly introduces the bacground of MALDI-TOF MS technology, including sample preparation and workflow. And we mainly discuss the application of MALDI-TOF MS in the identification of microorganisms and discuss the limitations and challenges of MALDI-TOF MS.

Poster Presentation : **ANAL.P-241**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Structural Studies of P143 in group C derived from IgG antigen Apo B-100 by NMR spectroscopy

Jieun Lee, GilHoon Kim[1], Hoshik Won[1,*]

The department of applied chemistry, Hanyang University, Korea

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

Apolipoprotein B-100(Apo B-100) which contains 4,536 amino acids was the main protein composed of LDL (Low density lipoprotein) and this serves to decompose cholesterol in the body by combining with LDL receptor. The oxidized LDL peptides by MDA (Malondialdehyde) or acetylation in vivo were act as antigen. These peptides were hard to interact with receptors and metabolic activity was suppressed. Therefore, it accumulated in the body and caused atherosclerosis. In vivo, the oxidized LDL peptides acted as antigen may generate immune response with the immunoglobulin (Ig). Apo B-100 were classified into 7 peptide groups (A to G) with subsequent 20 amino acids (p1-p302) according to the immune response specificity by oxidation of proteins with MDA and the ELISA (Enzyme-linked immunosorbent assay) analysis. The structural analysis studies of solution state p143 (IALDD AKINF NEKLS QLQTY) out of group C peptides carrying the high value of IgG antibodies after MDA oxidization were conducted. Signal assignment of p143 were carried out by homonuclear 2D-NMR(COSY, TOCSY, NOESY) using the NMRviewJ software and structural determination of p143 using DG(Distance geometry) and MD(Molecular dynamics) was performed using our programs(HYGEOM, HYNOE, HYNMR) with distance information between H-H atoms in each residues obtained by NOE signal assignment. The proposed structure was selected by comparisons between experimental NOE spectra and back-calculated NOE results from the determined structure showing acceptable agreement. Structural studies based on NMR may contribute to studies related to the prevention of LDL oxidation to prevent and treat atherosclerosis and to observing the conformational characteristics of Apo B-100 in LDL using monoclonal antibodies.

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Poster Presentation : **ANAL.P-242**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Analysis of the effects of NO gas in cancer cells based on NO-generating electrochemical system

Chae ri Park, Jeeyoung Ma[1], MyungKook Son, Dongjoon Im, Sooyeon Chae, Kyoungsuk Jin[2,*], Hugh I. Kim[*]

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

In vivo tissue activity control is achieved by delivering various physiological molecules between cells inside and outside the tissue. Therefore, when studying life phenomena and diseases at the molecular level, it is necessary to simultaneously analyze the interactions between biological molecules in cells and various organic and inorganic molecules and ions. However, a clear understanding is difficult due to the complexity of cell groups in the sample. Furthermore, studying the reactivity and adaptability of cells by external gas molecules is experimentally very limited. In this study, we applied an electrochemical system to control NO gas delivery to cells and investigated the effect of NO gas on cells by concentration. We placed A549 cells in a NO-generating electrochemical system and exposed these cells to NO gas. Distinct cell viability was observed based on the applied NO concentration. We also developed an available system to adjust the distance from cells to the NO-generating working electrode to control the degree of exposure to NO gas. Our results provide a materialized platform capable of observing the gas reactivity of cells by external gases to understand the cellular responses to gas molecules in the actual complex intracellular and extracellular microenvironments.

Poster Presentation : **ANAL.P-243**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Innovative mass spectrometer for high-resolution ion spectroscopy

Yu Ran Lee, Chan Ho Kwon[1,*]

Forensic Chemistry Division, National Forensic Service, Korea
[1]*Department of Chemistry, Kangwon National University, Korea*

Conventional ion spectroscopy is inapplicable for ions produced in low concentrations or with low spectral resolutions. Hence, we constructed a high-resolution vacuum ultraviolet mass-analyzed threshold ionization (HR VUV-MATI) spectrometer. This spectrometer is composed of a four-wave difference frequency mixing cell capable of generating long-lasting and intense VUV laser pulses of approximately 1 × 10^{10} photons/pulse at wavelengths of 123.6–160.0 nm, a space-focused linear time-of-flight photoionization chamber with a new ion-source assembly, and a compact molecular beam chamber with a temperature-controlled pulsed nozzle for ion spectroscopy. The ion source assembly and pulsing schemes enabled an approximately 15-μs-delayed but extremely weak pulsed-field ionization of the molecules in the zero kinetic-energy (ZEKE) states. These ZEKE states were effectively generated by a minute electric jitter from the high-lying Rydberg states that were initially prepared via VUV photoexcitation and first-order space focusing of the generated MATI ions. Enhanced spectral and mass resolutions of approximately 5 cm^{-1} and 2,400, respectively, were achieved using this spectrometer. Moreover, it could be used to measure the fine vibrational spectrum from the zero-point level of the cation and the exact adiabatic ionization energy of the neutral molecule. Additionally, it could be used to measure the appearance energies of the photoproducts and elucidate the vibrational structures of the cationic isotopomers, utilizing other pulsing schemes

Poster Presentation : **ANAL.P-244**
Analytical Chemistry
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One-pot synthesized FeSe quantum dots in an organic phase

Hyojin Kang, Youngeun Choi, Yujin Choi[1], Jae Kyung Lee[1], Jaebeom Lee[1,*]

Chemical engineering and Applied chemistry, Chungnam National University, Korea
[1]*Chemistry, Chungnam National University, Korea*

Quantum dots(QDs) are one of the most important achievements in nanotechnology. They have unique optical properties, for example, when their electrons are excited by receiving energy, QDs emit diverse colors depending on their sizes. Due to the properties of QDs, QDs have been successfully applied in various fields such as optics, electronics, and biology. Existing quantum dots use rare heavy metals and are expensive therefore they have limited applications. Herein, we described the one-pot synthesis of FeSe QDs in the organic phase for high quantum yield. The FeSe QDs exhibited a UV absorption band at 365 nm and a photoluminescence (PL) spectrum at 440nm and 460nm with a relative quantum yield of 56.4%. The QDs have an average size of 3.5 nm and a bandgap of 3.11 eV is observed. These results will suggest a way for the industrial application of FeSe QDs.

Poster Presentation : **ANAL.P-245**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Structural Characteristics of Functional Polysaccharides by Negative Tandem Mass Spectrometry

Sanggil Lee, Hyun Joo An*

Graduate school of analytical science and technology, Chungnam National University, Korea

Naturally-derived polysaccharides are in the spotlight as new biomaterials of the future. In particular, fucoidan extracted from the extracellular matrix of brown algae with high potential as a new material is a type of sulfated polysaccharide containing fucose that has various biological activities such as anti-coagulant and anti-cancer properties. These biological functions of fucoidan are closely related to their physical properties such as sulfate content, position, monosaccharide composition, and molecular weight. Here, we determined the structural diversity of fucoidan using MALDI-TOF/TOF MS and LC-MS/MS. Fucoidan was extracted with hot water and fractionated according to acidity by AEX chromatography to get rid of alginate, laminarin, and other contaminants. To facilitate the unit structure analysis of fucoidan, the purified fucoidans was hydrolyzed with mild acid to produce low molecular weight fucoidans, which were further purified by PGC-SPE. We profiled backbone chain composed of sulfate containing-head groups and fucose-repeated unit using MALDI-TOF MS. Hetero-oligomeric fragments separated by PGC were analyzed to be composed of sulfated fucose and monosaccharides unit such as hexose, uronic acid, and xylose by LC/MS. Sulfate positions of fucoidan were elucidated by negative CID tandem MS. For instance, the 0,2X fragment ion at m/z 139 and 0,2A fragment ion at m/z 183 from cross-ring cleavage by MS/MS indicate that sulfate groups are locacted at C2/C4 positions of the fucose. In order to understand the relationship between structure and biological activity, a multifaceted analysis is currently underway to elucidate the diversity of fucoidan structures. This work was supported by the National Research Foundation of Korea Grant funded by the Korean Government (MSIP) (2021, R&D Equipment Engineer Education Program, 2014R1A6A9064166).

Poster Presentation : **ANAL.P-246**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Identification and Analysis of Biomarkers from Novichok-inhibited Human Plasma

Woo-Hyeon Jeong

Chem-Bio Technology Center, Agency for Defense Development, Korea

NOVICHOK is a series of novel nerve agents reported firstly in Skripal Attack in 2018. We identified biomarkers from Novichok-inhibited human plasma for verification purposes. Butyrylcholinesterase and Human Serum Albumin were chosen for the target of biomarker identification using protease digestion and estimated the structure and exact mass of Novichok-inhibited biomarkers based on finding for conventional nerve agents. We successfully detected biomarkers for verification against Novichok in human plasma, and their MS2 Spectra was assigned and utilized for further analysis of OPCW Biomedical Proficiency Test (BioPT) or authentic plasma samples.

Poster Presentation : **ANAL.P-247**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Assessment of health risk under exposure of airborne particulate matter in mouse by LC-MS based metabolomics

Seungwoo Seo, Tae-Young Kim[*]

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

In this study, liquid chromatography-mass spectrometry based metabolomics was performed on mouse model exposed to airborne particulate matter (PM). Exposure group mice were injected with PM by intratracheal instillation. Metabolites were extracted from the heart and the lung of exposure and control group mice. Partial least-squares discriminant analysis was conducted on the abundance of differentially expressed metabolites to examine whether exposure of PM caused difference in metabolite profiles between the two groups. Biological impact of PM exposure on mice was tracked by annotating metabolic pathways associated with differentially expressed metabolites. Common and unique biological implications between the two organs were also investigated, to evaluate total adverse effects on the cardiopulmonary system. This study suggested important metabolic changes resulting from PM exposure, which can be utilized to elucidate its toxicity mechanism.

Poster Presentation : **ANAL.P-248**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of ultrathin Ni–Fe LDH nanosheets for efficient electrochemical water oxidation

Goddati Mahendra

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

Abstract: In an electrochemical water splitting, developing a cost-effective, abundant and highly efficient electrocatalyst is a major challenge for the large-scale production of hydrogen and oxygen gasses. Recently, applications of transition-metal based layered double hydroxides as electrocatalyst in water splitting have attracted attention because of their abundance, stability and environmental friendliness. An ultrathin nickel-iron layered double hydroxide (NiFe-LDH) nanosheet was synthesized using electrodeposition onto nickel foam (NF) substrates. In alkaline solution, the as-synthesized ultrathin nanosheet has exhibited an excellent oxygen evolution activity. Combined with its lower overpotential of 240 mV at 10 mAcm-2, turnover frequency at an overpotential of 400mV, and durability over 15, 000 s, this material is a promising electrocatalyst for water splitting.

Poster Presentation : **ANAL.P-249**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of graphene oxide with highly preserved sp^2 carbon network as an efficient matrix for Laser Desorption/Ionization Time-of-Flight Mass Spectrometry

Seung-Woo Kim, **Young-Kwan Kim**[1,*]

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

Matrix-assisted laser desorption/ionization time-of-flight mass spectrometry (MALDI-TOF-MS) has been widely adopted for analyzing large molecular weight compounds such as peptides, proteins, nucleic acids and polymers. However, MALDI-TOF-MS cannot be applied directly to analysis of low molecular weight compounds due to the interference from the conventional matrix. Graphene oxide (GO) has been used as a matrix for matrix-free laser desorption/ionization time-of-flight mass spectrometry (LDI-TOF-MS) analysis to overcome this drawback. Unlike GO synthesized by Hummers' method (HGO), the commonly used in LDI-TOF-MS analysis, GO synthesized by modified Brodie's method (BGO) has highly preserved sp^2 carbon network and less defective structure. Here, we systematically compared HGO and BGO as a matrix for LDI-TOF-MS analysis of various analytes such as small molecules and synthetic polymers. The LDI mechanism on HGO and BGO was also explored by using a model thermometer molecule. Based on the results, we found BGO exhibited a much higher efficiency in LDI-TOF-MS analysis than HGO through the distinct LDI mechanism owing to its highly-preseved sp^2 carbon structures resulting in high laser energy absorption, photothermal conversion, thermal stability and conductivity.

Poster Presentation : **ANAL.P-250**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Study on the Development of Reference Materials for Quantitative Analysis of MIT/CMIT in Living Chemicals

Jimin Park, Nu Ri Seong, Woo Seok Choe, DeogJun Gwon, Yonghyeon Lee, Wonpyo Hong, Seung Hwan Lee, Harin Jeong, Tae Ho Yeom*

Product safety & hazardous substances evaluation center, Korea Testing & Research Institute, Korea

CMIT/MIT has been widely used as a powerful preservative in domestic chemicals. However, regulations are being enforced across households due to strong inhalation toxicity. Related manufacturers need standard materials to check the contents and contents of CMIT/MIT in raw materials and finished products. A reference material must have the same or similar medium as a sample to compensate for the effect of the medium. Surfactants and spices are used as the main ingredients of cleaning agents, and various raw materials such as surfactants, fatty acids, waxes, diluents, preservatives, and spices are used for cosmetics. CMIT/MIT is developed by pro-nuclear attacks and is greatly affected by pH. In this study, the key goal is to create a chemical environment so that CMIT/MIT can exist reliably in cleaning agents and cosmetics media. Currently, CMIT/MIT standard substances in the form of living chemicals are not supplied at home and abroad. KTR is developing cosmetics cream preparation and cleaning liquid CMIT/MIT standard materials as a standard substance production agency and is planning to supply them to industries after 2023.

Poster Presentation : **ANAL.P-251**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Characterizing the Optical Properties of Hollow Gold Nanoshells with Plasmonic Effect

Yun a Hong, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

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

Poster Presentation : **ANAL.P-252**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

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

Seongeun Heo, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

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

Poster Presentation : **ANAL.P-253**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Study on the development of polyethylene certified reference material for bromine quantitative analysis

DeogJun Gwon, Yangseok Bhang, Kiyoung Heo, Yonghyeon Lee, Wonpyo Hong, HeeJin Lee, Tae Ho Yeom, Jimin Park, Jung Ae Park*

Product safety & hazardous substances evaluation center, Korea Testing & Research Institute, Korea

The regulation of hazardous substances among electrical and electronic products is spreading to developed and developing countries with the inception of the European RoHS (Restriction of Hazardous Substances Directive) and REACH (Registration, Evaluation, Authorization and Restriction of Chemicals). In particular, as the substances that account for a significant number of regulated substances are bromine (Br) compounds and chlorine (Cl) compounds, international requirements for halogen element regulation have increased, and accordingly, the international name “halogen-free” is being regulated. As the halogen regulation increases, the demand for the development of a certified reference material (CRM) for halogen analysis has increased, and halogen CRM is currently being developed and sold in several countries. Currently, domestic test institutes and global companies that perform halogen analysis are mainly using CRM from overseas brands, and accordingly, the need for developing domestic CRM dedicated to halogen analysis has emerged in order to reduce dependence on foreign countries. This study aimed to develop a certified standard material for quantitative analysis of bromine based on polyethylene (Poly Ethylene) material, which is widely used in electrical and electronic products. The target concentration was set at a high concentration of about 1,000 mg/kg and a low concentration of about 200 mg/kg. CRM candidate materials were developed through a series of procedures from production planning to manufacturing, homogeneity confirmation, stability confirmation, and characteristic value authentication. The results were calculated using the international standard (IEC 62321-3-2, Combustion-Ion chromatography), which is widely used internationally for halogen analysis.

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Poster Presentation : **ANAL.P-254**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Study on the mechanism and structure of LPcin analogs, antimicrobial peptides

Minseon Kim, Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Various organisms in nature have immune systems to protect themselves. Among the components of the innate defense system, antimicrobial peptides (AMPs) contain a large amount of cationic and hydrophobic amino acids, so they can be selectively destroyed by adhering to the anionic bacterial surface. Accordingly, research is being conducted to develop AMPs as therapeutic agents as way to overcome health threats caused by infections such as super bacteria and fungi.The AMPs we focused on is the LPcin-I derived from cow's milk, which is known to have antimicrobial activity against gram-positive and gram-negative bacteria and does not cause hemolysis of human red blood cells. Based on this LPcin-I, candidate peptides with improved antimicrobial properties were derived through peptide engineering and expressed in large quantities using bacteria to obtain high purity through an optimized separation and purification method. The mechanism of action of AMPs is known to kill bacteria through the 'barrel-state', 'carpet' or 'toroidal-pore' mechanism. Therefore, Solution/solid-state NMR spectroscopy and SEM were used to investigate the correlation between the expressed LPcin-analogs (YK peptides) and the membrane. In particular, using solid-state NMR, the structure and topology of peptides in the membrane environment were identified and the mechanism of action was studied.

Poster Presentation : **ANAL.P-255**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Dynamic Nuclear Polarization of Selectively 29Si Isotope-Enriched Silica Nanoparticles

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

Department of Bionano technology, Hanyang University, Korea
[1]*Department of Bionano Technology, Center for Bionano intelligence Education and Research, Hanyang University, Korea*
[2]*Department of Applied chemistry, Hanyang University, Korea*
[3]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*
[4]*Department of Bio-Nano Engineering, Department of, Korea*

Silica nanoparticles have garnered attention as promising biomedical probes for hyperpolarized 29Si magnetic resonance imaging and spectroscopy. We have demonstrated a straightforward method of synthesizing selectively 29Si enriched nano-sized silica particles with high degrees of control in terms of the particles' physicochemical properties and size. By utilizing 100% 29Si enriched TEOS, a silica precursor, selective enrichments on either particle surface (10 nm thickness) or core (40 nm diameter) were precisely conducted. With the particles of various structural characteristic, dynamic nuclear polarization (DNP) properties ranging from buildup, enhancement factor, and depolarization time at a cryogenic temperature were examined. The best considerable signal amplification was achieved from the silica nanoparticle with a selective enrichment localized on the particle surface, exposing both the successive surface polarization and polarization profile. The synthetic strategy with selective enrichments on the particles may expand the practical applicability of the nano-sized silica materials in various biomolecular processes, including targeted molecular imaging in vivo.

Poster Presentation : **ANAL.P-256**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Optimization of expression and structural studies of tIK peptides with anti-inflammatory activity

Jinhee Jeong, Minseon Kim, Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Rheumatoid arthritis, an autoimmune disease that causes inflammation around joints and damages ligaments and cartilage, spreads inflammation to the skin and blood vessels, causing headaches, anemia, and, in severe cases, vasculitis. This disease results from an imbalance between pro- and anti-inflammatory cytokines. Recent studies have found that truncated-IK (tIK) protein suppresses the expression of inflammatory cytokines. Therefore, we conducted a study to develop a therapeutic candidate peptide using only the region expressing anti-inflammatory properties among the amino acid sequences of the tIK peptide. We investigated phosphorylation patterns in macrophages of tIK transgenic mice and found that tIK protein phosphorylates tyrosine 496th of the interleukin (IL)-10 receptor subunit alpha in the mice without inflammation. To find the specific amino acid sequence part of the tIK protein that caused phosphorylation of the IL-10 receptor, the structure of tIK was predicted by comparing it with IL-10 using sequence homology modeling, and as a result, four epitope candidate groups were determined. By comparing the anti-inflammatory activity of each epitope through the T_H17 cell differentiation test, it was found that the 18 amino acid epitope had the best anti-inflammatory properties, and the peptide was named tIK-18mer. Based on this peptide, shorter anti-inflammatory 9-mers and 14-mers were also found.Peptides uniformly labeled with ^{15}N were expressed by culturing *E. coli* and the experimental purified procedure was optimized to analyze by MALDI-TOF and NMR. The secondary structure of the peptide was studied using CD and 2D NMR, and the interaction between the receptor and the tIK series was studied using chemical shift perturbation. Finally, an anti-inflammatory test was performed to confirm the anti-inflammatory effect of the purified peptide.

Poster Presentation : **ANAL.P-257**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Investigation of the structure of transmembrane protein syndecan-4 using NMR spectroscopy

Hyunjin Ko, Minseon Kim[1], Yongae Kim[1,*]

Chemistry, Hankuk University of Foreign Studies, Korea
[1]*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

The syndecan family is heparan sulfate proteoglycans, which consist of a core protein and heparan sulfate. Among the syndecan family, syndecan-4 is a type of transmembrane protein that transmits stimulation to cells through PIP_2 (phosphatidylinositol-(4,5)-bisphosphate) phospholipids. Syndecan-4 has an extracellular domain composed of (ecto-), transmembrane (TM), and cytoplasmic (Cyto-) domains, and an intracellular domain composed of C1, V (variable region), and C2 domains. The 183^{th} residue of syndecan-4, serine, is dephosphorylated to activate PIP_2 and activate protein kinase Cα. Activation of protein kinase Cα activates hormone binding and cytoplasmic calcium, which is involved in promoting tumor growth. The part that directly binds to PIP_2 is the V region, and the signaling process occurs through the cell surface receptor protein in the transmembrane domain, and the ligand binds to form a dimer.This protein is difficult to manufacture because it is a transmembrane protein that crosses the lipid bilayer of the cell membrane. We demonstrate an optimized method for expression, purification and NMR measurement of three types of syndecan-4 (wild-type Syd4-TM (wtSyd-4), mutant Syd4-TM (mSyd-4) and Sydecan4-eTC (Syd4-eTC)). To know the structural characteristics of the cell membrane region, three types of Syndecan-4 were expressed and purified with the amino acid sequence of the cell membrane region. To demonstrate the interaction of Syd4-eTC with PIP_2, the expression and purification processes were optimized and investigated by solution/solid-state NMR spectroscopy. The structure and orientation were investigated in the bicelle environment.

Poster Presentation : **ANAL.P-258**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fabrication of Home-built NMR Probes for Structural Studies of Various Samples

Jihong Wang, Minseon Kim, Yongae Kim*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Solid-state NMR has been steadily growing in popularity since the invention of NMR. Although solid-state NMR lacks inherent resolution compared to solution-state NMR, it provides many insights into organic and inorganic chemistry and serves as a power tool to study the local dynamics, kinetics, and thermodynamics of various systems. Many factors in each NMR assembly determine the performance of an NMR spectrometer among which the probe is the interface between the sample and the spectrometer. Above all, it is important to select probes suitable for various samples in order to obtain correct results in NMR experiments. Therefore, we manufacture the elaborate solid-state NMR probes for diverse sample analysis such as characterizing membrane proteins and defining of molecular dynamics in high tech devices.Here, we present the optimized design, construction, and efficiency of a home-built 400 MHz wide-bore (WB) & narrow bore (NB) ^{1}H-^{15}N double-resonance NMR probe and a home-built 800 MHz NB ^{1}H-^{15}N NMR probe for biological samples. In addition, a 400 MHz ^{1}H-^{31}P double resonance NB probe for studying the mode of action of antimicrobial peptides was fabricated. This study also describe home-built 400 MHz and 500 MHz NB ^{19}F-^{13}C NMR probes for *in situ* analysis of Li ion battery pack samples and 600 MHz NB ^{19}F-^{7}Li NMR probes with solenoid coils for irradiating Li ion batteries.

Poster Presentation : **ANAL.P-259**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

A Simple and Selective Detection of Micobial Toxin by Using Personal Glucose Meter for Point-of-care Testing

Junghun Park

Advanced Mechatronics R&D Group, Korea Institute of Industrial Technology, Korea

Microcystins (MCs), one of the most common microbial toxin, are a class of hepatotoxins detected in river, reservoir, and freshwater. MCs are monocyclic heptapeptides produced by cyanobacteria genera. In this study, we developed a simple and selective microcystin detection method based on personal glucose meter (PGM). This detection method was mediated by sequential enzymatic reactions including protein phosphatase, protein kinase, and hexokinase. In this study, we selected microcystin-LR as a target microcystin because of the highest toxic in the microcystins, and microcystin-YR and microcystin-RR for a selectivity tests. Through the developed sequential enzymatic reaction, in the absence of microcystin-LR, personal glucose meter (PGM) signal showed high level. However, in the presence of microcystin-LR, PGM signal showed low level. As a result, microcystin-LR can be selectively quantified against other microcystins by using PGM signal. Since this method does not require labeling and is completed within 60 minutes, this method can be applied to point-of-care testing (POCT).

Poster Presentation : **ANAL.P-260**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Identification and separation study of MGO trapping components from Volcanic rock processed green tea (VGT) using off-line HPLC

Kang Hyuk Kim, Soon Sung Lim*

Hallym University, Korea

Methylglyoxal (MGO) is an important precursor of Advanced Glycation End Products (AGEs) and can lead to diseases such as aging and diabetes.Green tea and tea polyphenols, including catechins, have been reported to have MGO trapping agents.However, there was no study on the MGO capture potential and composition of volcanic rock processed green tea (VGT) in Jeju. In a study to find non-toxic capture agents of reactive dicarbonyl species from dietary sources, a small number of bioactive green tea polyphenols, some catechin-related polyphenols (CRPs), efficiently trap reactive dicarbonyl compounds (MGO or GO). It has been discovered that a single substance can be formed. CRP bound at different ratios inactivated MGO (or GO) was analyzed using LC/MS. We also developed a method to purify materials that inactivate MGO in CRP without derivatization, and their structures were confirmed based on 1D and 2D NMR spectra.Our LC/MS and NMR data showed that it is the main active site for capturing reactive dicarbonyl compounds. In this study, the purified MGO trapping material could be used as a standard for further in vivo studies.

Poster Presentation : **ANAL.P-261**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Investigation of Oxygen Plasma Treatment Effect on Au@AuHg alloy Nanoparticles

Jaeran Lee, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

This study shows oxygen plasma treatment effect of Au@AuHg alloy core-shell nanoparticle for the structural, localized surface plasmon resonance (LSPR) spectral, and surface Au atom distribution changes. Au@AuHg alloy nanoparticles subjected to different plasma treatment times were characterized using transmission electron microscopy (TEM) and total internal reflection scattering(TIRS) microscopy and spectroscopy. The mercury ion solution treatment for 3 hours changed AuNR to Au@AuHg alloy spherical particles, and the thickness and atomic ratio of the shell and core was confirmed through TEM. The AR of the single Au@AuHg alloy was decreased by structural deformation, while their LSPR linewidth was increased with increasing plasma treatment time. But the three-dimensional (3D) orientations of the particle showed non-variation tilt angles with oxygen plasma treatment . The results show that the shape of the AuHg alloy shell deformed close to spherical shape through oxygen collision, but did not induce deformation of the Au core in the process of the oxygen plasma treatment. Therefore, this study provides a deeper understanding of energy transfer distance by oxygen collision through plasma treatment of Au amalgam shell nanoparticles.

Poster Presentation : **ANAL.P-262**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Pilot study for biomarker discovery of prostate cancer using proteomics

Miseon Jeong, **Wonryeon Cho**[*]

Department of Chemistry, Wonkwang University, Korea

Prostate-specific antigen (PSA) is a protein biomarker used in the early diagnosis of prostate cancer (PCa) in clinics. However, the PSA level is elevated not only in PCa but also in other prostate diseases, resulting in false-positive diagnoses. This pilot study aims to discover biomarkers that enable a more accurate early diagnosis of PCa by detecting PSA from prostate tissues in PCa patients and then identifying the proteoforms of PSA specific to PCa. However, there is difficulty in detecting PSAs present in trace amounts among abundant proteins present in tissues. First, the proteome was profiled by applying shotgun proteomics to a prostate tissue from the PCa patient with a high blood PSA level, and the PSAs were identified. After that, we intend to investigate PSAs in the tissue of PCa patient whose blood PSA level is in the gray zone of 4-10 ng/mL and compare the proteome of prostate cancer tissues also. Further study will be the targeted proteomics which captures only PSAs in PCa tissues.

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Poster Presentation : **ANAL.P-263**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Liquid Chromatography-Tandem Mass Spectrometric Analysis of Toxicants in Household Chemical Products

Hyeonjeon Cha, Woo Young Song, Tae-Young Kim*

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

Non-target screening analysis using high performance liquid chromatography-ultrahigh resolution mass spectrometry (MS) was performed in an attempt to identify toxic chemicals in four household chemical products, including bleach, fabric softener, synthetic detergent, and washing machine cleaner. Across the four household chemical products, 3043 features were detected using Compound Discoverer and 30 chemicals were tentatively identified by NIST 20 database and mzCloud MS/MS spectral library. Among the tentatively identified 30 chemicals, 11 were found in public chemical information database with their toxicity information: dermal toxicity for (–)-caryophyllene oxide, triethanolamine, 4-methoxybenzaldehyde, triethyl citrate, 2-hydroxy-4-(octyloxyl)benzophenone, ethylvanillin, and methyl dihydrojasmonate and oral toxicity for 4-hydroxybenzaldehyde, 6-aminocaproic acid, and (E)-alpha-ionone.

Poster Presentation : **ANAL.P-264**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Efficacy of Natural Antibacterial Feed in Paralichthys Olivaceus using Proteomics

Junghoon Kang, Youngjin Kim, Wonryeon Cho[*]

Department of Chemistry, Wonkwang University, Korea

Antibiotics and chemotherapeutics have been frequently used to treat bacterial infection in order to prevent mass mortality in aquaculture products such as Paralichthys olivaceus (P. olivaceus). However, these compounds may eliminate beneficial bacteria and produce antibiotic-resistant pathogenic strains, and thus remain as residues in the human body. This study aims to analyze the efficacy of antibacterial feed by detecting proteome alteration of P. olivaceus after feeding antibacterial feed, which is being developed using natural amino acids generated from animals and plants. One group of P. olivaceus was fed antibacterial feed while another group was fed general feed for four weeks, and then both groups were artificially infected with Streptococcus parauberis. Proteins were extracted with RIPA buffer from homogenized head kidney tissues of both P. olivaceus groups. Then each supernatant fluid was trypsin digested and desalted respectively. After that, the proteins in both groups were identified with nLC-MS/MS and protein database searches. Proteins were significantly identified only in the group fed with antibacterial feed, and the efficacy of the antibacterial feed was analyzed by performing protein functional analysis.

Poster Presentation : **ANAL.P-265**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Diabetes Type Distinction Based on Integrated Nanogap

Aejin Lee, Jong Kwan Park, Dong Hun Kim, Cho Yeon Lee, Wan Soo Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Integrated nanogap for the quantification of c-peptide was fabricated for the use in the diabetes type distinction. It is important to determine the types of diabetes because treatment should depend on the type of diabetes. Type 1 and 2 diabetes can be distinguished by quantifying c-peptide, a byproduct of insulin production. For the c-peptide quantification, sandwich immunoassay using gold nanoparticles and magnetic particles was adopted along with the integrated nanogap. In this way, C-peptide concentration was quantified in the range of 10^(-11) ~ 10^(-5) M,, which was adequate for the type distinction.

Poster Presentation : **ANAL.P-266**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Electrochemical Detection of Creatinine for Calibration of Urine Sample Concentration

Dong Hun Kim, Jong Kwan Park, Aejin Lee, Wan Soo Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Electrochemical quantification of creatinine was conducted to be used as an internal standard to correct the concentration of biotargets in urine. Creatinine is a substance produced by muscle activity that is produced by the body at a constant rate. Therefore, it is suitable as a standard material for concentration correction. Quantitative analysis was performed by the signal change in cyclic voltammetry after reacting an electroactive material with creatinine. Creatinine in urine was quantified in the normal range of 3.3×10^{-3} to 2.7×10^{-2} M.

Poster Presentation : **ANAL.P-267**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

[Withdrawal] PCR-Free Detection of BKV DNA Using Integrated Nanogap Sensor

Park So yeon

chemistry, Sungkyunkwan University, Korea

Poster Presentation : **ANAL.P-268**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Electrochemical biosensor for Influenza A H1N1 with multiple amplification strategy

Jonghwan Lim, Sanghyeon Park, Seunghun Kim, Eun Bin Kang, Wan Soo Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Multiple amplification strategy was devised for the improvement of the detection limit of electrochemical biosensor for influenza A. Electrochemical measurement by nanogap interdigitated electrode (nIDE) was combined with immunoassay using enzyme-linked polystyrene bead (PSB). Narrow gap in the nIDE facilitates the redox cycling of a probe molecule, giving an amplified electrochemical current, and the PSB increases the number of enzymes generating the probe molecule. In other words, the nIDE enhances the signal current at a fixed probe concentration, while the PSB raises the probe concentration at a fixed reaction time. As a result, limit of detection was extensively improved from 103 pM to 50 fM, compared to ELISA.

Poster Presentation : **ANAL.P-269**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

PCR-Free Detection of BKV DNA Using Integrated Nanogap Sensor

Park So yeon, Wan Soo Yun[1,*]

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

Since BK virus causes a serious problem upon kidney transplant, devising a simple detection method of its gene is one of the important diagnostic issues. In this work, detection of extremely low concentration of BK virus DNA was demonstrated using an integrated nanogap sensor without relying on DNA amplifying techniques such as PCR. The limit of detection of about 1 fM was readily attainable, which is well below the cut-off value of BK virus diagnosis (~16 fM), and the dynamic range was found to be about 105 (1 fM - 100 pM).

Poster Presentation : **ANAL.P-270**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Electrochemical Sensor for Aspergillus niger Based on Extracellular Protein

Semee Kim, Seunghun Kim, Sung Ik Yang[1], Wan Soo Yun*

Department of Chemistry, Sungkyunkwan University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Aspergillus niger (A.niger) was electrochemically quantified in the filtrate of the fungus solution with the use of a surface-functionalized micro/nano-gap interdigitated electrode (IDE). When the antibody in the gap region of the IDE captures the antigens, or extracellular proteins, the redox cycling of electrochemical probe was hindered and the current was reduced. Since the extent of current reduction should be a function of the antibody-antigen binding, it provides a good measure of the antigen concentration and also the A.niger concentration. It was found that the detection limit of our sensor was about 10 spores/mL, when ~500 nm gap IDE was used.[1] Jisu Lee, Semee Kim, Ha Young Chung, Aeyeon Kang, Seunghun Kim, Heeyoun Hwangm Sung Ik Yang*, Wan Soo Yun*, Journal of Hazardous Materials 411, (2021) 125069

Poster Presentation : **ANAL.P-271**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Long-term Effects of Exposure to Microplastics at Environmentally Relevant Concentrations on Lipidome of the Mouse Heart and Brain

Jonghyun Kim, Tae-Young Kim*

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

Most studies on the toxicological effects of microplastics (MPs) have been limited to a relatively short-term duration under high concentrations which are irrelevant to human exposure conditions. To overcome the limitation, this study investigated the long-term effects of MP exposure at environmentally realistic concentrations on the mouse cardiac and brain lipidome. The concentrations of MPs were determined based on the reported abundances of MPs in foods and their daily consumptions. In the consideration of size-dependent absorption of MPs through the digestive system, only MPs with size less than 10 μm were exploited for the experiments. MPs were orally administered to mice via drinking water for 1, 3, and 6 months. Relative quantification of lipids was carried out by deuterium oxide labeling for global omics relative quantification (DOLGOReQ). To reveal the relationship between quantitative change of lipids and the exposure conditions including exposure period, size, and polymer type of MPs, statistical analysis using ANOVA for the exposed groups was performed. Our results implied that the reported toxic effects of MPs could have been overestimated due to the use of excessively high concentration of MP.

Poster Presentation : **ANAL.P-272**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Reusable Electrochemical Microgap Sensors for Detection of Influenza A Virus Nucleoprotein

Sanghyeon Park, Jonghwan Lim, Eun Bin Kang, Seunghun Kim, Wan Soo Yun*

Department of Chemistry, Sungkyunkwan University, Korea

Reusable electrochemical sensors were fabricated for the detection of nucleoprotein (NP) from the influenza A virus. To maximize the number of reuses and lower the detection limit at same time, the reaction that forms sandwich structures with target NP was separated from the sensor. This separation was accomplished by immobilizing antibodies for target NP to magnetic particles, not sensor surfaces. By this way, the sensors could be used more than 20 times and the detection limit was found to be about pM of NP.

Poster Presentation : **ANAL.P-273**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Integrated Nanogap Sensors for Electrical Quantitation of Pathogenic Antigen

Cho Yeon Lee, Seokcheol Kim[1], Wan Soo Yun[1,*]

Nano/Bio Fusion Technology Research Center, Sungkyunkwan University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Nanogap sensors are a useful tool for biomolecular detection due to their considerable advantages such as simple fabrication process, easy measurement, high sensitivity, design flexibility of electrodes and high on/off current ratio. In many cases, biosensors using the nanogap device have led to electrical conductance change derived by gold nanoparticle (AuNP) probes between the two electrodes owing to presence of target biomolecules. However, conductance value is often unpredictable and random, weakly correlated with the concentration of targets, making it difficult to quantitate them with nanogap devices. In this work, we introduce a new method for the quantitation of target antigens by digital domain analysis, where the fraction of signal-on-device, or on-device-percentage (ODP), was translated into the concentration of the target molecule based on integrated nanogap sensors. The ODP was found to be closely related to the number density of the AuNP probes and, therefore, is an excellent measure of the target concentration. In addition, the results of quantifying antigens at ultra-low concentrations using passive and active-type of integrated nanogap sensors will also be discussed.

Poster Presentation : **ANAL.P-274**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Quantitative Detection of BKV Virus Using Toehold-Mediated Strand Displacement Reaction Based on Integrated Nanogap Sensor

GyeongYeon Byeon, Seokcheol Kim, Park So Yeon, Wan Soo Yun*

Department of Chemistry, Sungkyunkwan University, Korea

A selective quantitation for the BK virus DNA was investigated by combining integrated nanogap and Toehold-Mediated Strand Displacement (TMSD), a method of exchanging one strand of DNA with another. When DNA-modified AuNPs were exchanged by the target DNAs, the released AuNPs was quantitatively measured by the integrated nanogap. The results were discussed with the data from electrophoresis, SEM, UV/vis, DLS, AFM and electrical characterization. This study is expected to be utilized in the development of simple clinically-useful sensors.

Poster Presentation : **ANAL.P-275**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Quantitative analysis of phospholipid in Krill Oil using 31P-qNMR

Eun Jeong Shin, Sangdoo Ahn[1,*]

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

qNMR which stands for “quantitative analysis”, refers to an NMR technique used to determine the concentration of one or more chemical species. Since the signal obtained from NMR measurement is directly proportional to the concentration of atomic nuclei in the same environment of the molecule to be observed, the concentration of the molecule can be determined by comparing it with a standard material. qNMR is widely used in research in various organic matter-related fields including medicine, food or natural product because the sample preparation process is very simple, and there is no direct standardization process. Also, quantitative information can be obtained only by comparing the sample alone or with a standard material. Using the qNMR methods, in this research, we have performed the quantitative analysis of phospholipid in krill oil. We determined the chemical shift of phospholipid based on the chemical shift of TPP(Triphenyl phosphate), an internal standard of 31P-qNMR. The content of phospholipid in krill oil was calculated using qNMR equation.

Poster Presentation : **ANAL.P-276**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Comparison of volatile compounds in domestic Doenjang and imported Doenjang samples using headspace GC-MS

Hanbyeol Jang, Jeongkwon Kim*, Jina Lim

Department of Chemistry, Chungnam National University, Korea

Doenjang is a traditional fermented soybean paste food widely consumed in Korea. In order to secure the quality of Doenjang, a reliable analytical method is necessary. Here, we optimized headspace GC-MS conditions for a successful analysis of Doenjang samples. The Doenjang samples for current investigation are domestic Doenjang and imported Doenjang, which are sold in the market. For the headspace GC-MS analysis, lyophilized Doenjang samples (0.3 g) were put into a 20 mL headspace vial without pretreatment. Then, the volatile compounds were analyzed. As a result of preliminary experiments, a total of 37 volatile compounds were identified, including ketone, acids and esters, aldehydes, alcohols, furan, pyrazines. In order to solve the problem of broad peaks appearing at the beginning of the retention time, the split ratio was increased from 5:1 to 10:1. The other optimum conditions included m/z range of m/z 33 to m/z 350 and GC oven temperature of 40 °C for 5 min, increased at 10 °C/min to 200 °C, then held there for 5 min. In further study, we plan to perform quantitative analysis by adding an internal standard.

Poster Presentation : **ANAL.P-277**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Exploring Site-specific Glyco-heterogeneity on Horseradish Peroxidase by Multi-dimensional Approach using LC-MS/MS

Jaeho Kim, Hyun Joo An*

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

Plant-derived biotherapeutics are emerging in recent years because of their advantages over mammalian systems in terms of their large-scale production capacity, lack of animal pathogen contamination, and low cost of biomass production. However, relatively few studies have been conducted on glycosylation related to efficacy, stability, and safety in plant-derived biotherapeutics. From an immunogenicity point of view, the plant-derived biotherapeutics contain non-human glycosylation that should be monitored. Horseradish peroxidase (HRP) is a glycoprotein with high similarity to the glycan structures found in Taliglucerase alfa (TGA), the first plant-derived biotherapeutic approved for use in humans. Therefore, we proceeded with a comprehensive characterization of the glycosylation of HRP as a plant-derived biotherapeutic model. Herein, we applied a step-by-step strategy for the assessment of glycosylation quality for HRP at the intact protein, glycopeptide, and glycan levels. Various glycoforms and site occupancy were readily determined through intact protein analysis, and structural diversity was identified through glycan analysis. In particular, glycopeptide analysis using C18 UPHLC MS/MS allows to achieve in-depth site-specific glycosylation with micro & macro glycan heterogeneity. Non-human glycan moieties such as Xyl and Fuc (α1-3), were characterized at the glycan level. Site-specific microheterogeneity on eight glycosylation sites on HRP with nine glycosylation sites was observed using a glycopeptide analysis. Interestingly, through an intact level, fully occupied glycoproteoforms of the ninth glycosylation site were distinguished. This platform can utilize understanding in the N-glycan structures and glycosylation heterogeneity of plant-derived biotherapeutics.

Poster Presentation : **ANAL.P-278**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

A global and phosphoproteomic analysis of IDH1 mutated cell-line for investigation of the role of IDH1 mutation in GBM progression

Jiwon Hong, Sang-Won Lee*, Chaewon Kang[1], Su-Jin Kim

Department of Chemistry, Korea University, Korea

[1] *Korea University, Korea*

Glioblastoma multiform (GBM) is an aggressive type of cancer which occurs in the brain or spinal cord. Interestingly, a genome-wide mutational analysis revealed the association of survival increase and IDH1 mutation, a common mutation shown in GBM patients. However, extensive proteomic research regarding this mutation has not yet been systematically reported. Here we performed comprehensive proteome profiling on a IDH1 R132H point mutated cell-line to investigate the effect of the mutation on the progression of GBM.Using wild type, day1(early) and day 6(late) samples of two different cell-lines, three replicates of 6-plex TMT labeled peptides were obtained. Proteome profiling using DO-NCFC-RP/RP-MS/MS platform [2016, Lee *et al*] resulted in averages of 51,595 distinct phosphopeptides (41,603 phosphorylation sites, 7,352 phosphoprotein groups) and 259,061 distinct peptides (11,868 protein groups). GOBP analysis on the differentially expressed proteins and phosphorylation was carried out to investigate the early and late response signals by the mutation

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Poster Presentation : **ANAL.P-279**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Colorimetric Detection for Receptor Binding Domain of SARS-CoV-2 virus for Developing Paper-based Immunoassay

Xiaoyue Xu, In Geol Choi[1,*]

Department of Biotechnology, Korea University, China
[1]*Department of Biotechnology, Korea University, Korea*

AbstractSince the COVID-19 caused an outbreak in December 2019, millions of people in the world have been infected with the virus because of its high speed of transmission and the number of infections is still increasing, regardless of vaccination. The most common diagnostic method used in clinics is RT-PCR because it is the most accurate method but time-taking. Fast, simple, accurate and self-available diagnostic methods have been explored constantly to avoid infection. To develop a Do-It-Yourself (DIY)) diagnostic kit, paper-based colorimetric immunoassay was considered. This method is based on the interaction between antigen (RBD of SARS-CoV-2) and antibody (H11-D4). We employed Aryl Acylamidase (AAA) as a reporter that gives a color change. We cloned and overexpressed an antibody protein fused with AAA (H11-D4-AAA) to bind the spike protein of SARS-CoV-2. The binding affinity of H11-D4-AAA against RBD was determined as 131nM using surface plasmon resonance and the detectability also confirmed by dot blot assay. The detection limit of this colorimetric method was lower sensitivity than RT-PCR when the image analysis was applied (e.g. photographing using smartphone).Keywords: DIY, paper-based colorimetric immunoassay, SARS-CoV-2, aryl acylamidaseAcknowledgmentThis work was supported by Center for Women In Science, Engineering and Technology(WISET) grant funded by the Ministry of Science and ICT(MSIT) under the team research program for female engineering students.

Poster Presentation : **ANAL.P-280**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Quantum Dot Detection Probe of Nano-Biochip for Highly Sensitive Detection of Biomolecules by Total Internal Reflection Spectroscopy

Junghwa Lee, Seong Ho Kang[1,*]

Department of Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Unique photon properties of quantum dot (Qdot) make them a potential tool in the study of high-sensitivity detection of biomolecules. Herein, we evaluated the optical properties that Qdot can be used as a detection probe. In addition, differences in characteristics according to photobleaching, photostability, and intensity of different detection probes (Alexa fluorescent dye, plasmonic silver nanoparticle, and Qdot) on nano-biochips by total internal reflection spectroscopy. As a result, all three detection probes showed excellent specificity to biomolecules. In particular, plasmonic silver nanoparticle and Qdot exhibited greater resistance to photobleaching compared to the Alexa fluorescent dye, as well as better photostability and high signal-to-noise ratio, resulting in high detection sensitivity in evanescent field layer on nano-biochips. Qdot could be used as a nanoprobe to detect various biomolecules on biochip with high detection sensitivity and stability.

Poster Presentation : **ANAL.P-281**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Engineering and Identification of Marine Bioactive Peptide to Enhance the Properties of Antioxidant and Anti-inflammatory

Soyun Choi, Dong-Ku Kang*

Department of Chemistry, Incheon National University, Korea

It has been discovered that various marine active peptides have antioxidant and anti-inflammatory activities. QHGV (glutamine-histidine-glycine-valine), oyster-derived peptide has been widely investigated its’ anti-aging and anti-inflammatory functions. Here, QHGV peptide is modified by adding various naturally-derived phenolic acids, which has C-3 methoxy radicals or C-4 hydroxyl in aldehyde or benzyl alcohol. Five types of phenolic acids are selected to provide superior antioxidant effects and phenolic acids were conjugated at the end of N-terminus. Cellular ROS was more decreased by Phenolic acid-conjugated QHGV comparing non-modified QHGV and phenolic acid conjugated does not induce cellular toxicity in HaCaT cells. In addition, Phenolic acid induces collagen expression of mRNA and protein level in HaCaT cells. It has been also well-identified that oxidative-stress relates with inflammatory responses. Therefore, effect of phenolic acid conjugation was characterized on anti-inflammatory property of QHGV peptide. Results indicate that phenolic acid conjugation inhibits LPS-induced nitric oxide synthase (iNOS) and cyclooxygenase-2 (COX-2) in mRNA level. These results suggest that modification of phenolic acid provides additional and stronger biological activities on QHGV peptides.

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Poster Presentation : **ANAL.P-282**
Analytical Chemistry
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Maximization of chiral chromatography efficiency through temperature control

Danbi Eun, Jae Jeong Ryoo[1,*]

Dept. of Chemistry Education, Kyungpook National University, Korea
[1]*Department of Chemical Education, Kyungpook National University, Korea*

The separation of two enantiomers is very important in many scientific fields.[1] If the enantiomers are separated and the two separated peaks are far apart, it is because the interaction between the two enantiomers of sample and the chiral selector (stationary phase material in the chiral column) is good and shows a large separation factor value. In addition, when the base line of the two peaks of the separated enantiomers is clearly separated, it shows a large resolution value, is effective for mass separation of chiral compounds, and it is advantageous to obtain optically pure chiral compounds from a practical point of view.In this study, how effectively the separation was changed in terms of separation factor (a) and resolution (Rs) through manual temperature control in the separation of two enantiomers of a racemic mixture for five chiral compounds[2,3] (N-3,5-DNB-DL-Leucine, N-3,5-DNB-DL-Alanine, N-3,5-DNB-DL-Phenylalanine, N-3,5-DNB-DL-Valine, N-3,5-DNB-DL-Phenylglycine) using HPLC. Through this study, it was confirmed that the analysis efficiency can be significantly increased through simple heating/cooling in HPLC.[1] Ward TJ, Ward KD. Chiral separations: a review of current topics and trends. Anal Chem 2012;84:626–635.[2] Yu JJ, Ryoo DH, Lee JM, Ryoo JJ. Synthesis and Application of C2 and C3 Symmetric (R)-Phenylglycinol-Derived Chiral Stationary Phases. Chirality 2016;28:186-191.[3] Ryoo JJ, Kim TH, Im SH, Jeong YH, Park JY, Choi SH, Lee KP, Park JH. Enantioseparation of racemic N-acylarylalkylamines on various amino alcohol derived π-acidic chiral stationary phases. J Chromatogr A 2003;987:429-438.

Poster Presentation : **ANAL.P-283**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

GC-MS analysis of the metabolites in Doenjang samples

Jina Lim, Hanbyeol Jang, Jeongkwon Kim*

Department of Chemistry, Chungnam National University, Korea

In this study, the metabolites in Doenjang samples were extracted and analyzed using gas chromatography-mass spectrometry (GC-MS). For the extraction, a mixture of methanol-chloroform-water (4:1:3, v/v/v) was used where the supernatant was used for the following GC-MS analysis. Prior to the analysis of GC-MS, trimethylsilyl derivatization was performed to increase the volatility of the metabolites. As a result, organic acids (propanoic acid, oxalic acid, and 1,2,3-propanetricarboxylic acid), amino acids (valine, isoleucine, serine, threonine, proline, aspartic acid, and glutamic acid), sugars and sugar derivatives (xylitol, ribonic acid, inositol, galactonic acid, and others) were identified. By comparing the metabolites of Doenjang samples from different countries of origin, we seeks to establish a method for determining the origin of Doenjang samples.

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Analytical Chemistry
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Quantitative proteomic analysis of VPA chemical mouse ASD model reveals enrichment of RNF146 and Wnt/ β-catenin signaling

Wooyoung Eric Jang, Min-Sik Kim[1,*]

Chemistry, Kyung Hee University, Korea
[1]Department of New Biology, DGIST, Korea

Autism spectrum disorder (ASD) is a heterogeneous neurodevelopmental disorder where patients have impaired social behavior and communication, repetitive behaviors, and restricted interests. While there have been numerous attempts to understand the pathogenesis of ASD, there is still no concrete understanding of ASD at a molecular level. We perform a global-relative-quantification analysis of the proteome of the VPA-induced ASD mouse model and control mouse's prefrontal cortex brain tissue. Relative quantification method by implementing TMT-labeled LC-MS/MS proteomic method, we observe a difference in proteomic level resulting in a better understanding of ASD in the molecular proteome. Our analysis shows that VPA-exposed mice showed up-regulation in upper neuronal regional proteins compared to the control. The proteomic data support the previous finding that ASD patients physically have more upper neurons. The overexpression or proliferation of neurons is directly related to the VPA chemical effect on prenatal brain development and Wnt/ β-catenin pathways. In this study, implementing proteomic approaches with network analysis revealed the molecular function of RNF146 related to ASD. Among the differentially expressed proteins, RNF146 (E3 Ubiquitin-protein ligase) increase in VPA exposed mouse showed a highly significant effect on canonical Wnt/ β-catenin signaling pathways the β-catenin beta-catenin destruction complex. The increase in RNF146 expression ubiquitinates AXIN protein, inhibiting the β-catenin destruction complex, resulting in decreased phosphorylated β-catenin. The proteins like CREBBP, TCF4, and GSK3B showed significant changes that indicate disfunction of β-catenin destruction complex and activation of transcription factors. Using the ASD mouse behavioral mouse test and western blot analysis have validated that RNF146 relation with ASD. This study contributes to understanding the proteome differences between ASD and control, and in our findings, RNF146 showed a clear indication of molecular correlation to ASD.

Poster Presentation : **ANAL.P-285**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Lipidomic profiling in serum and liver tissue of mice with nonalcoholic steatohepatitis (NASH)

Jiaxin Geng, Youngae Jung[1], Geum-Sook Hwang[1,*]

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

Nonalcoholic fatty liver disease (NAFLD) has become a global health problem, affecting 25% adult population. NAFLD is a spectrum disease ranging from simple steatosis, to nonalcoholic steatohepatitis (NASH) and hepatocellular carcinoma (HCC). However, there is still not enough data for lipid alteration in the process of NASH. In this study, we examined the lipidomic changes in serum and liver tissue of mice (n=16) using ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC/QTOF-MS). Control and NASH groups were fed with chow diet (n=8) and NASH diet (n=8) for 3 weeks, respectively. Score plots derived from principal component analysis (PCA) showed separations between control and NASH groups. Total 14 classes of lipids were identified from LC-MS data and then Mann-Whitney test was used to show the alterations of lipids in serum and liver tissue. Free fatty acids (FFAs) such as poly unsaturated FAs (PUFAs) showed similar decreases in both serum and liver tissue in NASH group. On the other hands, phospholipids and glycerolipids differed in NASH group between serum and liver tissue. This study demonstrates that UPLC-MS/MS based lipidomic profiling is a useful tool in detecting characteristic changes at early stages of NASH in serum and liver tissue.

Poster Presentation : **ANAL.P-286**
Analytical Chemistry
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Lipidomic analysis to evaluate effects of AMPK activation in diet-induced NASH mice

Yeajin Ju, Jueun Lee, Geum-Sook Hwang[*]

Western Seoul Center, Korea Basic Science Institute, Korea

Non-alcoholic steatohepatitis (NASH) is a risk factor for hepatocellular carcinoma accompanied by liver cell damage and inflammation along with fatty deposition. AMP-activated protein kinase (AMPK) plays an important role in controlling energy homeostasis and the activation can inhibit NASH pathology. However, the effect of the AMPK activation on hepatic metabolic rewiring is unclear. This study aimed to investigate the therapeutic effects of AMPK on hepatic metabolism on NASH using lipidomic analysis. C57BL/6J male mice were fed a choline-deficient high fat diet (CD-HFD) for 6 weeks to induce NASH and treated them with YE-21, a new direct AMPK activator candidate, every 2 days for 14 times. Then, we performed lipidomic profiling of liver tissue using ultra-performance liquid chromatography–quadrupole time-of-flight mass spectrometry. Mice were divided into four groups: control (n=12), YE-21 (n=12), CD-HFD (n=12), and CD-HFD+YE-21 (n=12). As a result of multivariate analysis, partial least squares-discriminant analysis (PLS-DA) score plots showed different lipidomic patterns between the CD-HFD and CD-HFD+YE-21 groups. Eleven and thirteen classes of lipid metabolites were identified in positive and negative mode, respectively. After YE-21 treatment, CD-HFD+YE-21 group, compared to CD-HFD group, had significantly higher levels of phosphatidylcholines (PCs) and phosphatidylethanolamines (PEs). In contrast, lower levels of diglycerides (DGs) and triglycerides (TGs) were observed in CD-HFD+YE-21 group than CD-HFD group. Interestingly, TGs with long acyl chains (>50 carbon atoms) were significantly increased in CD-HFD mice compared to control mice and then significantly decreased after YE-21 treatment, whereas there was no change in TGs with short acyl chins after YE-21 treatment. These data suggest that AMPK activation induces low levels of TGs, which were associated with steatosis amelioration. This study demonstrates that lipidomic analysis is effective method to investigate AMPK effects on NASH.

Poster Presentation : **ANAL.P-287**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Determination of the Seed Contents of Red Pepper Powders by ^{1}H NMR and FT-IR Spectroscopy

Hyunjin Kwon, Sangdoo Ahn[1,*]

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

Red pepper powder is one of the representative spices in Asia, which is commonly used in Korean food. However, because domestic pepper powder is expensive, some manufacturers produce and sell low-quality red pepper powder by adding more seeds to increase the weight. Since any exact information about the seed content is not provided, consumers cannot discriminate whether it is the real red pepper powder. Also, it is not easy to judge by appearance alone. Therefore, an accurate technique is needed for determining the seed content of red pepper powder.In this study, FT-IR spectroscopy and NMR spectroscopy are used to determine the seed content of red pepper powder. In the FT-IR and ^{1}H NMR spectra, 30 variables of ^{1}H NMRR and 26 variables of FT-IR were differed by seed content. Then 18 variables of ^{1}H NMR and 3 variables of FT-IR were selected as signals which has greatly determining ability using Canonical discriminant analysis one-way analysis of variance (ANOVA) test. Finally, a regression model was completed by selecting one variable each from ^{1}H NMR and FT-IR through multiple linear regression analysis. The ability of the discriminant variable was verified through a blind test using a statistical technique, and the result was confirmed as meaningful data as the content of red pepper seeds showed a difference of less than 10% from the original group.

Poster Presentation : **ANAL.P-288**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Efficient and High-throughput proteomic analysis by fully automated Dual online reverse-phase liquid chromatography

Chaewon Kang, Soo Hyun Jung[1], Hye-Kyeong Kwon, Sang-Won Lee[*]

Department of Chemistry, Korea University, Korea
[1]*Department of Nanobio, Gachon University Global Campus, Korea*

The large number of proteome samples entails a fast method utilizing a short gradient reverse-phase liquid chromatography with no dead time in between experiments. In this study, we developed a simple dual online reverse-phase liquid chromatography system for high-throughput proteome analyses. This simple system employ two additional switching valves (two position four port valve) on a single LC system utilizing two binary pumps. This system is fully automated and offers many advantages such as high duty cycle, high separation resolution, and high reproducibility. In contrast with the single LC system, the dual online reverse-phase liquid chromatography system equipped with two analytical columns effectively removes the dead time for column wash and equilibration. As a result, this system can provide an increase in experimental throughput by two folds, while keeping the reproducibility between two analytical columns. With this system, we optimize 10 minutes gradient with high flow rate in order to perform 144 analyses per day. Therefore, the fully automated dual online reverse-phase liquid chromatography system is ideal for high-throughput MRM experiments, involving a large cohort sample.

Poster Presentation : **ANAL.P-289**

Analytical Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Effect of Glutathione Injection on Thermal stress in Olive flounder Based on the Metabolomics

Seonghye Kim, Juyoung Choi, Youzhen Li, Suhkmann Kim*

Department of Chemistry, Pusan National University, Korea

The increases in water temperature disturb homeostasis and induce oxidative stress in aquatic organism. Supplementing with glutathione (GSH), a major intracellular antioxidant, can be effective in relieving stress. In this study, we elucidated the effect of GSH on olive flounder (Paralichthys olivaceus) exposed to high temperature using serum parameters and NMR-based metabolomics. In the results of first experiment, 20 mg of GSH was identified as an effective dose. For the experiments of thermal stress, fish were divided into 3 groups; Control, Temp (PS injection), and GSH (glutathione injection). The temperature in Temp and GSH groups were increased from 20 °C to 27 °C. The results of serum parameters did not change significantly, but the deviation in Temp group was greater than that in GSH group. Based on the metabolomics results, Temp group was clearly distinguished from the control and GSH groups in OPLS-DA score plots of the kidney. In the liver, the metabolic patterns of GSH group were close to the Temp group on day 4 and became similar to Control group from day 7. The levels of GSH, lactate, O-phosphocholine, and betaine in the kidney and levels of taurine, glucose, and several amino acids in the liver were significantly altered in Temp group compared to control. These metabolites were related to antioxidant activity and energy system. Therefore, these results provide the effect of GSH injection relieving thermal stress influencing metabolic mechanisms in fish.

Poster Presentation : **ANAL.P-290**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Wavelength-dependent light-sheet-based non-fluorescence super-resolution microscopy for three-dimensional superlocalization and real-time single-particle tracking

Yingying Cao, Seong Ho Kang[1,*]

Chemistry, Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

Wavelength-dependent light-sheet-based super-resolution microscopy (LSRM) for precise three-dimensional (3D) superlocalization and single-particle tracking (SPT) of anisotropic plasmonic nanoparticles has been developed. This imaging technique combined wavelength-dependent scattering, simultaneous dual-wavelength detection with dual-view, and astigmatism method for real-time superlocalization and SPT in 3D. To accomplish this, gold nanorods (AuNRs) as anisotropic plasmonic nanoparticles were illuminated by a light-sheet to reduce photodamage and increase signal-to-noise ratio. The individual AuNRs could be detected at an imaging rate of 100 frames per second with the localization precision of ~6 nm laterally and ~14 nm axially. By comparing the widths of the experimental point spread function of AuNRs with the corresponding calibration curves, the 3D spatial coordinates of AuNRs could be resolved in real-time. This 3D LSRM imaging technique could be applied for real-time 3D tracking and superlocalization of biomolecules in live cells at subdiffraction limit resolution.

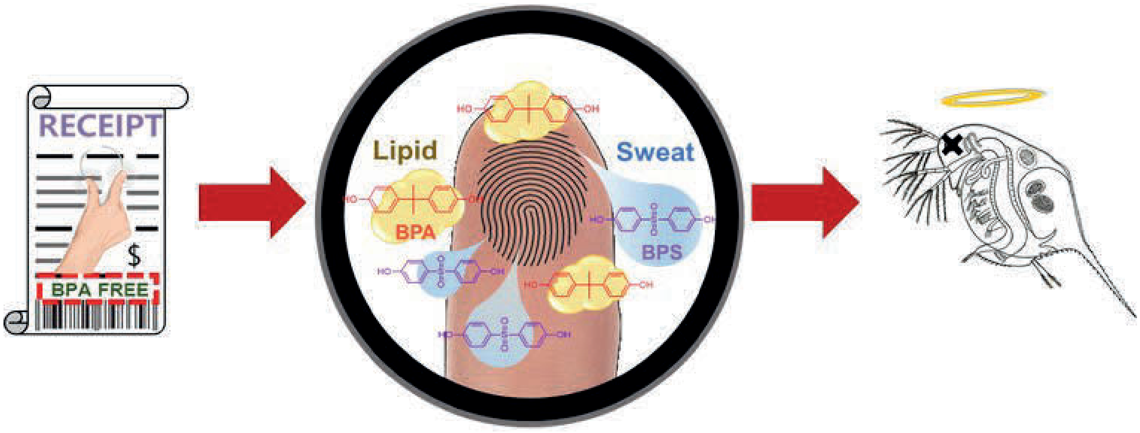
Poster Presentation : **ANAL.P-291**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

The risk of dermal exposure of BPA-free materials

Min Jang

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

Bispheonl A (BPA) is still being found in a wide array of manufactured products including thermal papers, plastic water bottles, canned foods, and pacifiers despite reported toxicity of BPA to human beings. BPA is also a frequently used monomer in engineering plastics. Therefore, consistent requests of BPA replacement have been surged. Bisphenol S (BPS) is one of replacements and BPS containing materials (receipts and colored papers) are sold in the market labeled as BPA-free. However, is it actually safe?This research reported that BPS is present in BPA-free labeled materials with enormous amount (10000 and 500 μg/g, respectively). Since they are handled by human beings in daily basis, BPS can be transferred to human skin. Our newly developed liquid chromatography mass spectrometry (LC-MS) method qualitatively and quantitatively detected BPS (5 to 26 μg/g) as well as BPA (28 to 89 μg/g) in fingerprints. Furthermore, using a matrix assisted laser desorption ionization mass spectrometry image (MALDI-MSI) method confirmed visually the presence of BPS in a fingertip after a receipt handled, and that presence of sufficient oily materials without handwashing can pick up more amount of BPS than with handwashing. The level of BPS in fingerprints was then applied to the toxicity test using water flea. As a result, chronic exposure to BPS in spite of low concentration still adversely influenced on the birth and health of water flea. It means that chronic handle of BPA-free materials can be a big threat to the health system.


RECEIPT
$
BPA FREE
Lipid
Sweat
BPA
BPS
HO
OH

Poster Presentation : **ANAL.P-292**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

^{1}H NMR-based metabolomics approach to elucidate tissue-specific effects of RBIV infection in Oplegnathus fasciatus

Sujin Lee, Yujin Lee, Seulbin Ha, Hani Lee, Suhkmann Kim*

Department of Chemistry, Pusan National University, Korea

Rock bream iridovirus (RBIV) is a double-stranded DNA virus belonging to genus Megalocytivirus and occurs typically in the summer when the temperature of water is rise. It leads to severe mortality of Rock bream (Oplegnathus fasciatus) and vast economic losses in the aquaculture industry. Since this pathogen spreads quickly, rapid diagnosis for infection in fish is necessary. However, there are no studies investigating the physiological responses in fish infected to RBIV. In this study, rock bream was naturally infected with RBIV for 3 weeks. Based on the viral loads in the spleen at different sampling time point (0 and 3 week), control (0C), heavy-infected (0H) at 0 week and light-infected (3L) at 3-week groups were divided. The metabolic changes of liver, spleen, and kidney for each group were measured using High Resolution-Magic Angle Spinning Nuclear Magnetic Resonance (HR-MAS NMR). In liver and spleen, it was observed that RBIV utilized host cellular metabolism for its replication by increasing in metabolites related to energy production such as TCA cycle and Warburg effect. In the spleen and kidney, branched chain amino acids (BCAA) metabolism that involved in the host defense mechanism altered depending on the degree of RBIV infection. This study provides novel insights into the cellular metabolic pathways affected during iridovirus infection and a valuable resource for determining detailed mechanisms of host-pathogen interaction.

Poster Presentation : **ANAL.P-293**
Analytical Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Size Determination of Iron Oxide Nanoparticles Using Modified Single Particle ICP-MS

Jimin Shim, Heung Bin Lim[*]

Department of Chemistry, Dankook University, Korea

One of the most important concerns in the semiconductor production process is particle contamination management. For this, various techniques, such as SEM, TEM, and ICP-MS, have been used in the field. Among them, ICP-MS provides a lot of potential to achieve the purpose since it has outstanding capability for reliable quantification, size distribution and particle concentration determination. Iron oxide particle is one of the frequently observed contaminants in the manufacturing process. Nevertheless, it is difficult to determine it due to severe polyatomic interference and poor sensitivity in ICP-MS.The size estimation model recently developed in our lab showed excellent correlation of the integrated area of the peak to the cubic of Au particle radius through the data analysis based on Window Peak Selection and Gauss Fitting. In this work, iron oxide (Fe_2O_3) nanoparticles was studied for further proof and practical application. Since aggregation was extremely critical for the iron oxide nanoparticles, which deteriorated the accuracy of size determination, the influence of sonication time was seriously evaluated for the sample preparation. As the sonication time increased, the FeNPs were dispersed well in the solution, but their average intensity of the peaks tended to be decreased due to the appearance of many low intensity peaks caused by particle cracking. Therefore, the sonication time was optimized at 15 min for 5 and 10 nm and 5 min for 30 nm of FeNPs. The developed size estimation model showed good correlation of known particle size with corresponding integrated peak area, of which the obtained regression coefficients of R^2 were in the range of > 0.987. The obtained correlation function of $y = ax^3 + b$ or $\sqrt[3]{y}=ax+b$, can be used as a tool for fast determination of unknown particles in the process, indicating the great opportunity for on-line monitoring. In order to achieve such a high performance in the production line, blank subtraction and uncertainty of calibration process was inevitably studied, so the developed method can achieve high reliability and eventually apply to control the particle impurities in the semiconductor manufacturing process.

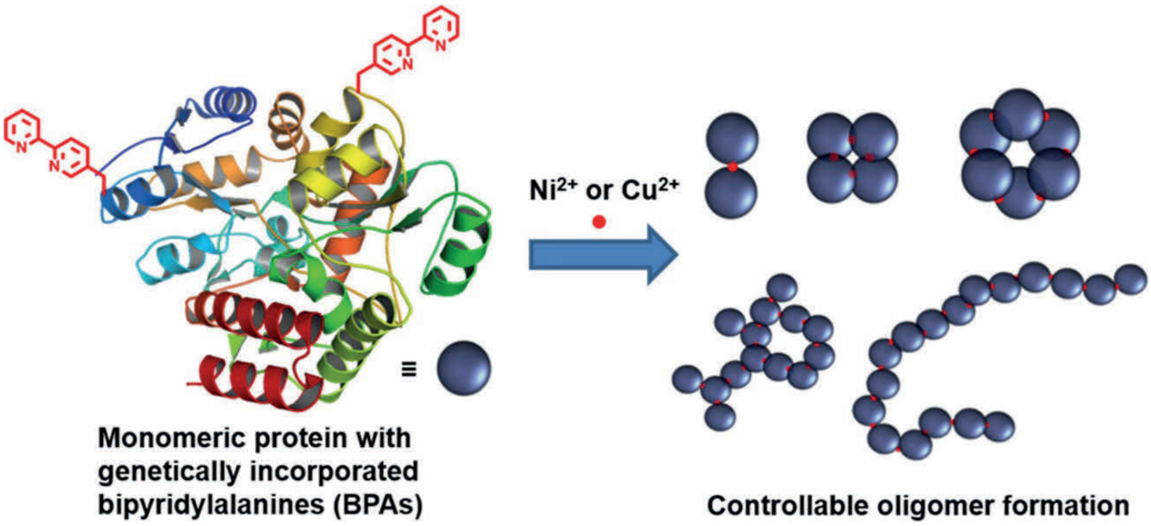
Poster Presentation : **LIFE.P-280**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Metal-Mediated Protein Assembly Using a Genetically Incorporated Metal-Chelating Amino Acid

Sooin Kim, Hyunsoo Lee*

Department of Chemistry, Sogang University, Korea

Many natural proteins function in oligomeric forms, which are critical for their sophisticated functions. The construction of protein assemblies has great potential for biosensors, enzyme catalysis, and biomedical applications. In designing protein assemblies, a critical process is to create protein–protein interaction (PPI) networks at defined sites of a target protein. Although a few methods are available for this purpose, most of them are dependent on existing PPIs of natural proteins to some extent. In this report, a metal-chelating amino acid, 2,2′-bipyridylalanine (BPA), was genetically introduced into defined sites of a monomeric protein and used to form protein oligomers. Depending on the number of BPAs introduced into the protein and the species of metal ions (Ni^{2+} and Cu^{2+}), dimers or oligomers with different oligomerization patterns were formed by complexation with a metal ion. Oligomer sizes could also be controlled by incorporating two BPAs at different locations with varied angles to the center of the protein. When three BPAs were introduced, the monomeric protein formed a large complex with Ni^{2+}. In addition, when Cu^{2+} was used for complex formation with the protein containing two BPAs, a linear complex was formed. The method proposed in this report is technically simple and generally applicable to various proteins with interesting functions. Therefore, this method would be useful for the design and construction of functional protein assemblies.


N
N
N
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Ni²⁺ or Cu²⁺
≡
Monomeric protein with genetically incorporated bipyridylalanines (BPAs)
Controllable oligomer formation

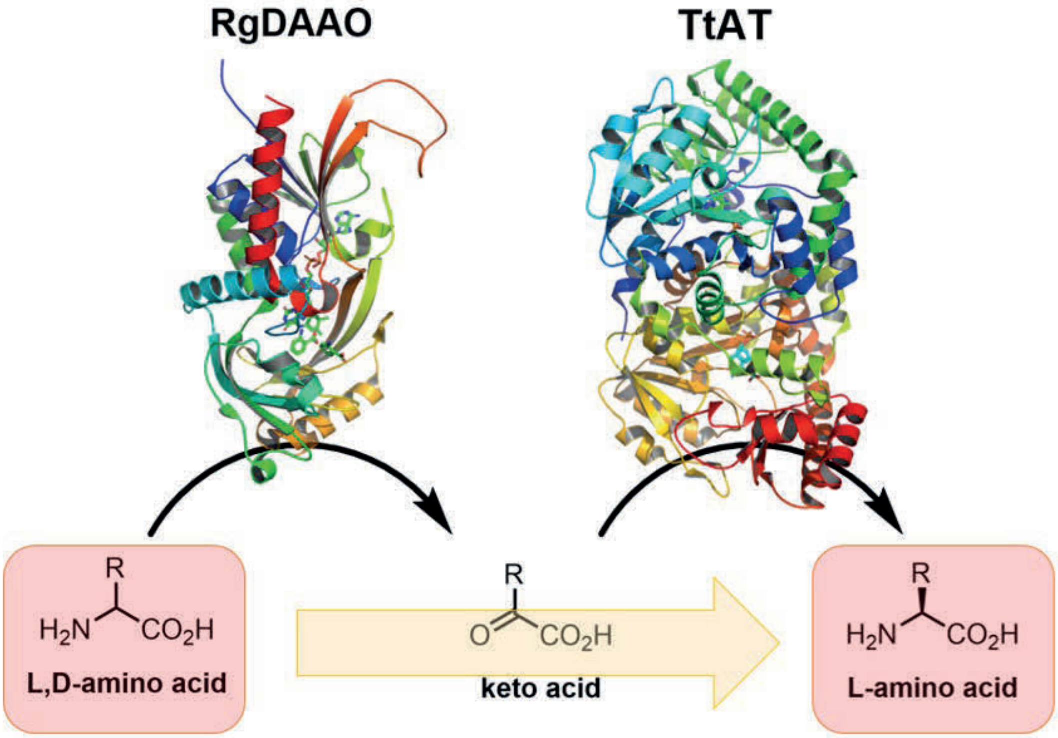
Poster Presentation : **LIFE.P-281**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Conversion of Racemic Unnatural Amino Acids to Optically Pure Forms by a Coupled Enzymatic Reaction

Sooin Kim, Hyunsoo Lee[*]

Department of Chemistry, Sogang University, Korea

Genetic code expansion (GCE) technology is a useful tool for the site-specific modification of proteins. An unnatural amino acid (UAA) is one of the essential components of this technique, typically required at high concentration (1 mM or higher) in growth medium. The supply of UAAs is an important limitation to the application of GCE technology, as many UAAs are either expansive or commercially unavailable. In this study, two UAAs in a racemic mixture were converted into optically pure forms using two enzymes, the d-amino acid oxidase (RgDAAO) from Rhodotorula gracilis and the aminotransferase (TtAT) from Thermus thermophilus. In the coupled enzyme system, RgDAAO oxidizes the d-form of UAAs in a stereospecific manner and produces the corresponding α-keto acids, which are then converted into the l-form of UAAs by TtAT, resulting in the quantitative and stereospecific conversion of racemic UAAs to optically pure forms. The genetic incorporation of the optically pure UAAs into a target protein produced a better protein yield than the same experiments using the racemic mixtures of the UAAs. This method could not only be used for the preparation of optically pure UAAs from racemic mixtures, but also the broad substrate specificity of both enzymes would allow for its expansion to structurally diverse UAAs.


RgDAAO
TtAT
R
H2N
CO2H
L,D-amino acid
R
O
CO2H
keto acid
R
H2N
CO2H
L-amino acid

Poster Presentation : **LIFE.P-282**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Distinct Impact of Glycation towards the Aggregation and Toxicity of Murine and Human Amyloid-β

Eunju Nam, Mi Hee Lim[*]

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

Alzheimer's disease (AD) is characterized by the deposition of senile plaques primarily composed of human amyloid-β (hAβ). Modification of hAβ such as the formation of the advanced glycation end products (AGEs) is implicated to be involved in the accumulation of the amyloid plaques. In the brain of aged mice, murine Aβ (mAβ) which differs in three amino acid residues (Gly5, Phe10, and Arg13) compared to hAβ is less likely to form the amyloid aggregates. How the aggregation of mAβ and hAβ is disparate remains unclear, however. Herein, we report that the advanced glycated end products of mAβ_{40} over hAβ_{40} are distinctly generated. The different glycation between the two peptides can govern their aggregation kinetics, structural transition, and cytotoxicity. Our studies provide a better understanding of how the difference in the degree of glycation towards Aβ affects its aggregation and toxicity profiles.

Poster Presentation : **LIFE.P-283**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

A Preliminary Structure-Activity Relationship Study of NSAID Dimers as Multi-Acting Ligands for Neuroinflammation inhibition in Alzheimer's disease (AD)

Hyerim Ju, Sungwoon Choi[*]

Chungnam National University, Korea

Alzheimer's Disease (AD) is a multi-factorial neurodegenerative disease without known exact cause and neuroinflammation is one of the main event in the brain of patient afflicted with AD. Exposure to non-steroidal anti-inflammatory drugs (NSAIDs) was shown to reduce the risk of AD. Among NSAIDs cromolyn indicated for asthma as a master cell stabilizer with ibuprofen was shown to decrease the amount of Aβ by promoting microglial phagocytosis is under clinical trial for AD. Using cromolyn as a lead structure, naproxen-type and ibuprofen-type dimers were designed to generate multi-acting ligands especially targeting neuroinflammation modulation. A hydroxypropyl or propyl tether linked two of aryl propionic/carboxylic acids as pharmacophoric features common in cromolyn and NSAIDs resulting in dimeric structures. Dimeric NSAIDs were preliminarily tested for the transcription inhibition of inflammation related factors such as COX-2 and iNOS under cell-based assay. CNU-2 and 3 inhibited dose-dependently LPS-induced COX-2 and iNOS expressions at mRNA and protein level in BV2 cells. Even with no clear demonstrable SAR trends were identified, critical structural features necessary for neuroinflammation modulation was found. New analogs are under preparation and these will be a valuable asset for the pharmacotherapeutics and preventive agents against AD with further investigation.

Poster Presentation : **LIFE.P-284**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Development of Artificial Intelligence Model For Prediction of Drug Metabolite Site

Jee-Young Lee[*], Minwoo Han[1], Yuna Ha[1], Seungju Lee[2]

Structure-based Drug Discovery, Daegu Gyeongbuk Medical Innovation Foundation, Korea
[1] *New Drug Development Center, Daegu Gyeongbuk Medical Innovation Foundation, Korea*
[2] *NDDC, Daegu Gyeongbuk Medical Innovation Foundation, Korea*

By introducing ADME evaluation studies from the early stages of drug discovery, the failure rate in drug development due to bioavailability and pharmacokinetic characteristics has improved significantly from 40% to less than 8% since the 1990s. Analyzing and optimizing metabolic characteristics in the early stages of drug development is a major strategy that can reduce the time and cost required in the drug development process and increase the rate of success in drug development. Along with the development of computer hardware and artificial intelligence technology, various artificial intelligence studies have been conducted to predict drug metabolism. However, deep learning-based methods for metabolites prediction have not yet been developed. To develop a deep learning-based prediction model, it is necessary to build a high-quality metabolite database, use advanced algorithms, and train and verify artificial intelligence models.This study aims to collect drug metabolite data and develop an artificial intelligence model that predicts the metabolite of drugs. We built a database of metabolites based on the data we collected. To facilitate the collection and management of drug metabolism information, we developed a GUI-based information program to collect information on major metabolic reactions in published papers. The collected data was standardized based on major journals related to drug metabolism and various pathway information for small molecule compounds so that it could be easily used to develop an artificial intelligence model. To date, about 1700 drug metabolism-related literature and 5000 drug metabolism information have been collected and standardize and will be updated continuously.We are developing a deep learning-based model that predicts metabolites of drugs using the established metabolite data. The developed model will be used for model validation and advancement by conducting metabolite mass spectrometry experiments in parallel. Finally, the developed metabolism prediction model plans to build a web-based service platform so that researchers can use it for new drug development research.

Poster Presentation : **LIFE.P-285**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Efficient shRNA delivery to breast cancer overexpressing HER1 through multimeric rolling circle transcription products containing alternating HER1-against RNA aptamer and HER1-against shRNA units

Juhyun Jo, Sang Soo Hah*

Department of Chemistry, Kyung Hee University, Korea

In this study, we present the development of a new siRNA delivery method for enhanced gene silencing, which is based on HER1 RNA aptamer-mediated intracellular delivery of multimeric shRNAs. By making use of rolling circle transcription (RCT) in order to produce multimers containing alternating HER1-against RNA aptamer and HER1-against shRNA units, the multimeric RCT products were observed to show significant gene silencing effects leading to cell death, even without any additional delivery vehicles, in comparison with the conventional monomeric shRNAs and/or HER1-against RNA aptamers mixed with lipofectamine. Importantly, cell viability assays revealed that MDA-MB-231 cells with the highest expression levels of HER1 on the cell surface compared with HeLa and SK-BR-3 cells are the most sensitive to the multimeric RCT products. Our observations suggests that the introduction of RNA aptamer as delivery moiety of shRNA delivery system can allow specific and efficient target binding/removing as well as target gene suppression with persistent and druggable intracellular uptake capacity.

Poster Presentation : **LIFE.P-286**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Supramolecular polymerization using the host-guest interaction for the cancer therapy

Haewon Ok

화학과, Ulsan National Institute of Science and Technology, Korea

Supramolecular polymerization is consisting of noncovalent bonding. Noncovalent bonds are used to make large molecules such as proteins and nucleic acid, that is weaker than the covalent bond, but crucial for biochemical processes. Therefore, using the supramolecular polymerization, interfere in the biochemical process for induce the cell death. One of the supramolecular polymerization's characteristic is host-guest interaction. Host molecules are connected with the targeting the cancer cell, and guest for disassemble the molecules before making the polymer. In addition, using the characteristic of the host-guest interaction, can change the guest molecules depend on the concentration, only in the cancer cell. With change the guest molecules, that can assist for the polymerization in the selective cell. Therefore, when the guest change occurs, the polymerization is starting to make the large molecules with the noncovalent bonding, and that polymerization can induce the cell death.

Poster Presentation : **LIFE.P-287**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Liposomal Coronavirus model, combined with recombinant spike proteins

Hyun Park, Huong Thanh Nguyen, Kwanwoo Shin[1,*]

Chemistry, Sogang University, Korea
[1]*Institute of Biological Interfaces, Sogang University, Korea*

With the outbreak of the SARS-CoV-2 pandemic, the study of the Coronavirus is now emerging as the most important issue to be addressed. The infection route of the coronavirus, the mechanism of reaction with human cells, or the development of vaccines or therapeutics are all related to the unique biological structure and components of the coronavirus. Essentially, they are Nucleocapsid (N) protein, Membrane (M) protein, Spike (S) protein and Envelope (E) protein, membrane, and single positive-strand RNA present in the cytoplasm. Particularly, the coronavirus spike (S) protein is known to initiate infection by binding to a specific receptor on the surface of many human cells. Therefore, we attempted to make a liposomal model virus that could understand the biological behavior of the coronavirus by inducing the adsorption of the S-protein of this coronavirus to the surface of a liposome. Here, we constructed a SARS-CoV-2 model using polyhistidine-tagged (His-tag) recombinant proteins to obtain a controlled and ordered array of proteins on the surface of Ni-NTA functionalized liposomes. The His-tagged protein was strongly attached to the liposome surface, interestingly exhibiting the S-protein's antigenic activity. Since this virus model has no genetic material, there is no risk of infection, but this virus model is expected in various research fields such as diagnostic kit validation, virus entry mechanism, and development of new vaccine candidates.

Poster Presentation : **LIFE.P-288**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

RIG-I Mediated Innate Immune Stimulation by Chemically Synthesized Long Double-Stranded RNAs Is Structure- and Sequence-Dependent

Younggyu Kang, Jaejin Kim[1], Kyeongmin Lee[1], Dong-ki Lee[1,*]

Platform Technology Unit 2, OliX Pharmaceuticals, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Since RNA interference (RNAi) initiated by double-stranded RNA (dsRNA) was discovered, it has provided a great tool for life science research and opened a new era of nucleic acid therapeutics because of its potent and specific target gene knockdown. Since Tuschl et al. reported short dsRNA (19+2 nt) showed efficient mRNA degradation without triggering any innate immune response, long dsRNA over 30 bp has not been considered as a potential candidate for RNAi therapeutics due to innate immune response. However, long dsRNA used earlier in the immune stimulation studies mainly is composed of in vitro transcribed products, that have 5’ triphosphate, a crucial ligand of RIG-I. With the progress in the RNA synthesis facilities, we tried to re-characterize the innate immune stimulation using various chemically synthesized dsRNAs without the key 5’ triphosphate. Herein we designed 38/40~60 bp chemically synthesized dsRNAs targeting single- or dual-gene with blunt-ends or 3' 2-nucleotide overhangs. In this study, we show that longer than 38/40 bp chemically synthesized dsRNA with blunt-ends induced RIG-I mediated innate immune response. Especially, we figured out that not only the length of chemically synthesized dsRNA but also a certain dsRNA sequence motif, si-GFP is important for RIG-I activation. Furthermore, chemically synthesized dsRNA longer than 38/40 bp could show single- or dual-gene targeting in Dicer-independent manner. In conclusion, these results demonstrate that chemically synthesized dsRNAs longer than 38/40 bp with immunostimulatory dsRNA motif may be a novel nucleic acid therapeutics platform, simultaneously achieving RNAi and boosting innate immune response. Our finding expands the structural diversity of RIG-I ligands and provides a guide to develop a multi-functional RNA structure for therapeutic application.

Poster Presentation : **LIFE.P-289**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Collagen Fibrils Formation from Collagen-encapsulated Nanoliposomes using Electrical Stimulation

Albertus Ivan Brilian, Chang Ho Kim, Agustina Setiawati[1], Kwanwoo Shin*

Department of Chemistry & Institute of Biological Interfaces, Sogang University, Korea
[1]*Department of Life Science, Sogang University, Korea*

Collagen is one of the prominent scaffolding components of the extracellular matrix that can turn into collagen fibers through self-assembly mechanisms. Recently, we found that an electric field can stimulate the collagen fiber formation process in an acidic condition through the aggregation of tropocollagen. When applying an AC of 10 Hz-1 V, collagen fibrils with a 28 to 70 nm diameter appeared within 20 minutes in a 0.01M HCl pH three buffer solution. We designed an experiment to form collagen fibers at a targeted region by encapsulating collagen molecules in nano-sized liposomes (Lip-Col) and have confirmed that the fibrils were successfully formed. We infer that electric field induced the formation of electroporation and changed the surface charge of Lip-Cols and pH solution; hence, Lip-Cols were first aggregated, and then fibrils with a 33-73 nm diameter were formed into a matrix-like structure. The internalization study of Lip-Cols in human dermal fibroblast (HDF) cells was further investigated, and we found that Lip-Cols can effectively interact with the cellular membrane, resulting in collagen networks in extracellular matrix space. Finally, we found that Lip-Cols under electrical stimulation enhanced the biosynthesis of type I human collagen in HDF, indicating that these Lip-Cols can be utilized as a drug delivery system for anti-aging or wound healing agents.

Poster Presentation : **LIFE.P-290**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Visualization of mRNA transcription in Artificial Cell using click-chemistry

SeonMin Jeon, Hyun Kyung Choi[1], Kwanwoo Shin[*]

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

Replicating in the form of newly assembled mRNA from a portion of DNA known as transcription is an essential part of the central dogma in molecular biology. Recently, mRNA, which works as an intermediate transporter in the course of protein synthesis, is receiving great attention in the medicinal industry for the development of new drugs including COVID vaccines. In this study, we aimed to develop a method to visualize mRNA transcription in artificial cells without additional treatment such as cell lysis or washing. We used 5-Ethynyl Uridine (EU) as a nucleoside analog of an RNA labeling material and combined a fluorescent material via click chemistry for microscopic visualization. The EU labeled RNA and pro-fluorophores with azide-only fluorescence when forming triazole rings by copper(I)-catalyzed alkyne-azide cycloaddition (CuAAC) reaction. In this study, we designed experiments to find suitable conditions for the click reaction that could selectively visualize mRNAs by varying the concentrations of EU and CuAAC reaction mixtures.

Poster Presentation : **LIFE.P-291**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Artificial cellular model for cytoskeletal-membrane interaction with artificial photosynthetic organelle

<u>Sungwoo Jeong</u>, Seohyeon Min[1], Sungwoo Lee[2], Hyun Park[1], SeonMin Jeon[2], Chang Ho Kim[3], Kwanwoo Shin[2,*]

Research Institute for Basic Science, Sogang University, Korea
[1]*Chemistry, Sogang University, Korea*
[2]*Department of Chemistry, Sogang University, Korea*
[3]*Institute of Biological Interfaces, Sogang University, Korea*

In a cellular system, both the cytoskeleton and the membranes are under dynamic and complex networks to maintain their bioactivity. Generally, most of the researchers defined these bio-compartments' general functions and bioactivities through in vitro experiments. However, in vitro experiments are limited to understand the interactions and dynamic networks between the compartments in a cellular shape closed system. Furthermore, as several researchers continuously found differences between in vitro and closed system experiments, the researchers are developing the optimal closed system to understand cellular bioactivities further. Therefore, we designed and built an artificial cellular model that explains the several different networks and interactions between differently conditioned membranes and self-polymerizing cytoskeletal proteins (F-actin). The giant unilamellar vesicles (GUVs) contain artificial photosynthetic organelles, which generate ATP with light. We triggered and controlled the actin polymerization by light which controls the ATP production of the artificial photosynthetic organelles. As the cytoskeletal filaments grew in the GUVs, they protruded and interacted with the plasma membranes. The morphologies were different by the modified phase properties of the GUVs: ordered/disordered phases from saturated/unsaturated, charged/zwitterionic, or cholesterol-free/cholesterol-containing phospholipids. We divided the morphologies into three conditions, no interactions, interactions, and the creation of an inner crust. Our models are the cellular shape closed system, which shows the possibility of creating cellular morphological changes or motion with only the interactions between cytoskeletal proteins and membranes with controlled actin polymerization.

Poster Presentation : **LIFE.P-292**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

DNA Visualization Using Streptavidin-Fluorescent Protein

Yu Jin, Kyubong Jo[*]

Department of Chemistry, Sogang University, Korea

Visualization of single large DNA molecules is a powerful platform for obtaining genomic and biochemical information. Typically, organic fluorescent dyes such as oxazole yellow homodimer (YOYO-1) have been used for the visualization of single molecule DNA. However, contemporary organic dyes have several critical limitations, such as photo-bleaching and photo-induced DNA cleavage. As a solution, we previously developed fluorophore-bound DNA-binding chemicals 1 and fluorescent DNA binding proteins23. Although our new approaches have succeeded in overcoming the previous limitations, they still have some weaknesses that are likely due to their weak interactions, such as hydrophobic and electrostatic interactions. In order to improve both the binding affinity and the specificity, we have developed a novel DNA visualization approach based on the avidin-biotin interaction, which is known to be the strongest non-covalent interaction (Kd=10-15). We constructed plasmids containing streptavidin and various colors of fluorescent proteins such as Superfolder GFP, mScarlet, mNeonGreen, mKO2, YPet, AausFP1 and RRvT. To make DNA optical maps, we labeled DNA sequence-specifically with biotins and then stained it with streptavidin fluorescent protein (SA-FP). Furthermore, biotin-labeled nucleotides were incorporated on the DNA ends using TdT (terminal deoxynucleotidyl transferase) and then SA-FPs were attached to visualize the DNA termini. In summary, streptavidin-fluorescent proteins on biotin-labeled DNA could be a powerful tool for DNA visualization.

Poster Presentation : **LIFE.P-293**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Imaging the Binding between Chemical Drugs and Its Target Proteins inside Living Cells

Mi-Hee Jun, Yang Hoon Huh, Kyung-Bok Lee*

Center for Research Equipment, Korea Basic Science Institute, Korea

In this work, we demonstrated that binding between a chemical drug and its targets in the cytoplasmic region could be imaged in living cells by combining a technique of spatially localized protein expression and chemical inducers of dimerization (CIDs) method. To verify our approach, Dasatinib, a kinase inhibitor and multi-target drug (its main targets are non-receptor tyrosine kinases such as ABL and SFKs), was chosen as a model compound, and was modified with HaloTag-ligand. HaloTag technology is based on the covalent interaction between 34kDa HaloTag protein and its ligands. HaloTagged fusion proteins can be expressed using standard recombinant protein expression techniques. Once the fusion protein has been expressed, there is a wide range of potential areas of experimentation including enzymatic assays, cellular imaging, protein arrays, determination of sub-cellular localization, and many additional possibilities. Firstly, HaloTag protein was expressed in specific intracellular compartments (endosome and F-actin were used in this study) and Dasatinib's target kinases (GFP tag was fused) were expressed in the cytoplasmic region. After treatment with HaloTag-ligand modified Dasatinib drug, the co-localization of Dasatinib drug and its target kinase was observed in specific intracellular compartments. We believe that this method would be a useful platform for image analysis of binding between chemical drugs and their cytoplasmic targets within living systems. We are currently exploring other proteins and small molecules in protein–drug binding studies.

Poster Presentation : **LIFE.P-294**

Life Chemistry

Exhibition Hall 1 THU 11:00~12:30

The crystal structure of L-leucine dehydrogenase from *Pseudomonas aeruginosa*

Seheon Kim, Seri Koh, Jin Kuk Yang[*]

Department of Chemistry, Soongsil University, Korea

Leucine dehydrogenase (LDH, EC 1.4.1.9) is a NAD^+–dependent oxidoreductase that catalyze the reversible oxidative deamination of L–leucine and other branched–chain L-amino acids (BCAAs). LDH is widely used in the stereoselective production of BCAAs using a bioreactor. For the application in a wide range of fields, structural and biochemical characterization of the enzyme is important. Here we report the crystal structure of LDH from *P. aeruginosa* at 2.5 Å resolution, and the biochemical characterization by Michaelis–Menten kinetic analysis. Interestingly, the structure of *Pa*LDH exists as a dimer in the crystal lattice as well as in solution confirmed by SEC–MALS. The specific activity of *Pa*LDH is maximum at 60 °C and pH 8.5. The kinetic parameters for the substrates, i.e. NAD^+, leucine, isoleucine, valine, cysteine, were determined.

Poster Presentation : **LIFE.P-295**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

The efficiency of transmembrane protein reconstitution into artificial cellular vesicles

Seohyeon Min, Sungwoo Jeong[1], Hyun Park, SeonMin Jeon, Kwanwoo Shin[*]

Department of Chemistry, Sogang University, Korea
[1]*Research Institute for Basic Science, Sogang University, Korea*

The transmembrane protein in a living cell is a membrane protein that extends through a bilayer of lipid within the cell and acts primarily as a conduit for chemical material transport. Until now, several protein reconstitution protocols were developed and suggested to reconstitute transmembrane proteins into the artificial cellular membranes, but, the efficiency and stability of the membrane proteins in artificial cells still need to be further improved. In this study, we developed an artificial cellular model with microbial rhodopsin (as a model of transmembrane protein) to find a way to improve reconstitution efficiency. The efficiency of transmembrane protein insertion was measured by varying preparative conditions such as lipid compositions, cholesterol ratio, pH, temperature, and buffer conditions. To confirm the functional activity of rhodopsin in artificial cells, the expression of rhodopsin was measured using a pH indicator in the rhodopsin reconstituted liposome. This model may provide an optimal method for implementing various functions of transmembranes in artificial cell models.

Poster Presentation : **LIFE.P-296**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Observing Anisotropic Mechanics of Human Dermal Fibroblasts Using Confocal and STED Microscopy

Sang Ho Lee, Agustina Setiawati, Dayoung Jang, Chang Ho Kim[1], Kwanwoo Shin[*]

Department of Chemistry, Sogang University, Korea
[1]*Institute of Biological Interfaces, Sogang University, Korea*

Living cells undergo morphological changes under physiological conditions that cause cytoskeletal alignment, leading to anisotropic behavior. However, although the role of the cytoskeleton in changing cell shape in anisotropy is known, it has not yet been clearly visualized. We observed the anisotropic response of human fibroblasts (HDFs) in variously patterned fibronectin, which provides a unique microenvironment for adherent cells. HDFs attached to various surfaces were immunostained and observed with simulated emission depletion (STED) and confocal microscopy. The resolution enhancement allowed a clearer distinction when observing anisotropic behavior in both 2D and 3D scans. We observed that fibroblast anisotropic orientation is induced through interactions with intracellular fiber and cytoskeletal alignment.

Poster Presentation : **LIFE.P-297**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Physcion promotes melanin production in melanoma cells through the modulation of MSRA and TRP-2

Ah In Jo, Moon-Moo Kim*

Department of Applied Chemistry, Dong-Eui University, Korea

Hair graying is related to the decrease of melanin pigmentation. Melanin pigment hair is synthesized in melanocytes in hair follicles. Melanin production is decreased with age. The excessive accumulation of H2O2 in the hair follicle accelerates hair graying of black hair. The aim of this study was to examine the effect of physcion, an aromatic organic compound, which is an anthraquinone compound that occurs naturally in dripping sewage on melanin production in B16F1 cells. Physcion, also called parietin, is a cortical pigment that is the main component of pigments found in the roots of the genus Caloplaca, a secondary product of lichens, and the roots of Curled Dock. Recently, physcion has been reported to have anti-cancer, anti-inflammatory, anti-apoptosis and antioxidant effects. The effect of physcion on melanin production was investigated in the B16F1 cell line. Cytotoxicity assay was performed in the presence of physcion using MTT assay. Physcion at the highest concentration of 10 μM displayed cytotoxicity by about 20%. In addition, physcion treatment at 10 μM increased the melanin production by 27% compared to the blank group in live cells. Both Western blot assays and immunofluorescence staining assay showed that physcion increased the protein expressions of MSRA and TRP-2. These findings suggest that physcion could be available as a potential therapeutic agent for the prevention of hair graying.

Poster Presentation : **LIFE.P-298**

Life Chemistry

Exhibition Hall 1 THU 11:00~12:30

Hybridization of Multi Composite Extracellular Matrix for Specific Tissue Engineering

Agustina Setiawati, Sungwoo Jeong[1], Albertus Ivan Brilian[2], Sang Ho Lee[3], Kwanwoo Shin[3,*]

Sogang University, Indonesia
[1]*Research Institute for Basic Science, Sogang University, Korea*
[2]*Chemistry, Sogang University, Korea*
[3]*Department of Chemistry, Sogang University, Korea*

The extracellular matrix (ECM) is a connective fiber network supporting cells to live in their surrounding environment. In particular, in the basal region of skin tissue, a multi-component ECM, composed of fibronectin (FN), laminin (LN) and collagen (COL I), is formed in forms of fibers. This study harnessed the fibrillogenesis to mimic the multi-component extracellular matrix. We simultaneously and sub sequentially manipulated the ECM component network by micropatterning FN to control the architecture of hybrid ECM synthesis. We found that all of ECM molecules undergo fibrillogenesis on the micropattern to form a hybrid architecture. By controlling the concentration of deposited COL I, this study successfully engineered a COL I rich and COL I less ECM composite for specific mammary gland and liver cells. Mammary gland cells prefer to attach on COL I rich composite than COL I less composite, and vice versa. Taken together, our system enables tailored ECM composite for specific tissue engineering. Keywords: extracellular matrix, fibronectin, collagen, laminin, tissue engineering

Poster Presentation : **LIFE.P-299**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Characterization of intracellular protein-protein interactions by FRET imaging in living cells

Soojung Yi, Nam Ki Lee[1,*]

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

Protein-protein interactions (PPIs) play crucial roles in most biological processes. One of the most important parameters to characterize PPIs is the dissociation constant (K_D), which reflects the strength of PPIs. Measurement of K_D *in vitro* is relatively feasible since the concentration of proteins and their environment can be easily controlled. In contrast, it is challenging to characterize PPIs in intact cells due to cellular complexity. Despite these difficulties, the importance of investigating PPIs *in vivo* has been increasing because the two environments differ greatly. Here, we established three-channel fluorescence resonance energy transfer (FRET) imaging system and directly obtained K_D of PPIs in single living cells, which has been considered a challenging task. Identification of the PPIs in living cells can provide us with a better understanding of the intracellular environment.

Poster Presentation : **LIFE.P-300**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Cell Lysate-based Cell-free Protein Synthesis in a Lipid Phase Separated Giant Unilamellar Vesicle

Sungwoo Lee, Hyun Park, Sungwoo Jeong[1], Kwanwoo Shin[*]

Department of Chemistry and Institute of Biological Interfaces, Sogang University, Korea
[1]*Research Institute for Basic Science, Sogang University, Korea*

Cell-free protein synthesis (CFPS) based on cell lysate has many advantages over protein synthesis in vivo. In particular, the lack of cell walls allows direct manipulation of biochemical cascades that usually occur in the cytoplasmic space. Meanwhile, we recapitulate that when cell lysate is encapsulated in artificial cell membranes, it could be the ideal cytoplasm for artificial cells capable of protein synthesis. It was, however, difficult to implement CFPS reactions using the cell lysates due to the osmotic instability in the confined spaces provided by liposomes. Furthermore, previous studies suggested that the membrane pores continuously produced during the reaction allow essential small molecules to pass through, which means GUV is no longer an independent space. In this research, we developed and optimized the cell-lysate components and demonstrated the cell lysate-based CFPS system in a giant unilamellar vesicle (GUV). We adopted an emulsion transfer method to prepare the cell-lysate encapsulated GUV with high encapsulation efficiency. By applying ultrasound to the vesicles, it was possible to increase the homogeneity of the encapsulated cell lysis solution, and as a result, almost all GUVs showed sharp green and red fluorescence, demonstrating that the fabrication of artificial cells, which are feasible to synthesize various proteins inside using a lysate-based expression system. We further constructed robust GUVs with lipid phase separation, which enabled GUVs to keep their shape intact against unpredictable change of osmotic pressure and prevent them from forming transient defects in membrane. In this presentation, we will present the results of artificial cells encapsulating E. coli extracts synthesizing different proteins from a single cell-sized liposome.

Poster Presentation : **LIFE.P-301**

Life Chemistry

Exhibition Hall 1 THU 11:00~12:30

Effect of molybdenum disulfide on silver doped zinc oxide for antibacterial activity

Joonho Shin, Kwang-sun Kim[*]

Chemistry, Pusan National University, Korea

Since the advent of multidrug-resistant (MDR) bacteria, controlling infectious disease caused by pathogenic bacteria has become more difficult. In this scenario, nanomaterials like zinc oxide could be a good alternative antibiotic to against this problem due to its physiochemical properties. Furthermore, doping zinc oxide with silver has several antibacterial mechanisms, including the production of reactive oxygen species (ROS) and apoptosis. Moreover, the success of 2D material like graphene has sparked huge interest on other 2D material such as molybdenum disulfide (MOS2), a 2D transition metal dichalcogenide (TMD), due to its intriguing physiochemical properties, high biocompatibility and antibacterial activity. Here, we synthesized silver doped zinc oxide functionalized with molybdenum disulfide (AZM) to investigate the antibacterial activity. The material properties of the nanocomposites were characterized using X-Ray Diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and Transmission electron microscopy (TEM) analysis. The micro dilution method was used to determine the minimal inhibitory concentrations (MICs) of AZM utilizing gram-negative bacteria strains such *Escherichia coli* (ATCC 25922) and others. The AZM had good antibacterial activity and was more effective against *E. coli* (MIC = 62.5 g/mL) than MDR *E. coli* (MIC = 7.81 g/mL). As a result, the AZM has antibacterial properties and the potential to be used as a biomedical nano-weapon.

Poster Presentation : **LIFE.P-302**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Design and fabrication of pump-free microfluidic PCR devices for fast and point-of-care diagnostics

<u>Eunjin Huh</u>, So Jung Kim[1], Nayoon Pyun, Hyuckjin Lee, Oh-Sun Kwon, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea
[1]*Biomedical Engineering , University of British Columbia, Canada*

Polymerase chain reaction (PCR) is a well-known technique for cloning and amplifying specific DNA sequences and is an essential tool in many applications, including disease diagnosis and pathogen detection. Researchers have developed a variety of microfluidic PCR devices to obtain test results rapidly, but most devices require a bulky pump or motors. Also, most devices have a fixed PCR cycle, which makes it difficult for users to amend the cycle or temperature. We developed a gravity-driven rotary PCR device to maximize the advantages of microfluidic PCR and at the same time, minimize the mechanical disadvantages that require an external pump. The device is compatible with the 2-temperature, shuttling PCR protocol; one for denaturation of double-stranded DNA and the other condition for combined annealing and extension steps. We performed a preliminary heating test and observed that each temperature region was able to provide the appropriate environment for each PCR step. The device has a stepper motor that rotates the chip by +45 degrees and -45 degrees to repeatedly move the fluid in a chip. The fluid moves by gravity without a pump, allowing the heater and motor to be controlled with a miniaturized microcontroller. In this presentation, the design and preliminary test results will be presented.

Poster Presentation : **LIFE.P-303**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Decellularized ECM-hydrogel for 3D-printing fabrication of ear cartilage scaffold with improved biocompatibility

Jae eun Kim[*], Agustina Setiawati[1], Albertus Ivan Brilian, Kwanwoo Shin[2,*]

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

3D printing method has been an attractive method for artificial tissue engineering and regenerative medicine. Various tissues such as bone, skin, nerve, heart, liver and cartilage have been fabricated using 3D bio-printing and tested in vivo. Among them, ear cartilage regeneration is an important research area for patients with deformities in auricle. Ear cartilage scaffold has been fabricate using various methods, including full decellularized tissue scaffold, 3D-printing hybrid hydrogels scaffolds, or 3D-printing decellularized ECM(d-ECM)-derived hydrogel scaffold. It has been known that d-ECM components such as collagen, proteoglycan, fibronectin and laminins are essential biological and tissue-specific components for cell growth and decellularization makes fabricated scaffold cell-free, which reduces inflammation response. In this regard, this study aims novel formulation of biomaterials for ear cartilage regeneration by mixing d-ECM with GelMA and alginate hydrogel. This study shows that the addition of d-ECM improves cell viability on the 3D printed ear cartilage scaffold and furthermore offers the perspective of the fabrication of patient-specific ear cartilage by 3D bio-printing.

Poster Presentation : **LIFE.P-304**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Structural and functional characterization of N^6-adenine methyltransferase YfiC

Hyeonju Jeong, Jungwook Kim[1,*]

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

Transfer RNA (tRNA) undergoes various post-transcriptional modifications. N^6-methyladenosine (m^{6}A) is common in mRNA and rRNA in all species. In tRNA however, this modification is only found in bacterial tRNA^{Val}(UAC) at 37th position. In *E. coli*, *yfiC* gene was identified to encode an SAM-dependent methyltransferase, which modifies A37 of tRNA^{Val}(UAC). However, understanding of structure and catalytic mechanism of YfiC remains elusive. Here, we show *in vivo* and *in vitro* activities of *M. capricolum* YfiC and present the crystal structures of *M. capricolum* YfiC bound with and without SAH. *M. capricolum* YfiC displays unique substrate specificity and requires divalent metal for its catalytic activity, unlike its *E. coli* homolog. From this research, relationship between structure and function of YfiC is discussed.

Poster Presentation : **LIFE.P-305**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effect of hydrophobicity and cationic charge to the activity of mitochondria-targeting peptoids

Soyoung Kim, Jiyu Lee[1], Jiwon Seo[*], Jiyoun Lee[2,*]

Department of chemistry, Gwangju Institute of Science and Technology, Korea
[1]*Department of Next-Generation Applied Science, Sungshin University, Korea*
[2]*Global Medical Science, Sungshin University, Korea*

Mitochondria-targeting system are essential for the development of clinical medicine concerning mitochondrial-related diseases such as neurodegenerative diseases, cancer or diabetes. Peptoids (oligo-N-substituted glycines) are biocompatible peptidomimetics which presents similar physicochemical properties as peptides with an added advantage of *in vivo* stability arising from enhanced resistance to proteolytic cleavage. In particular, amphipathic peptoids are membrane-permeable. By modifying their cationic charges and hydrophobicity, the function of amphipathic peptoids could be readily changed according to the purpose of the use such as cell penetration, anti-cancer or antibacterial activity. Previously, we synthesized a series of amphipathic peptoids that showed potent cell penetration and mitochondrial localization without inducing significant toxicity. As an extension of the study, we designed new analogs with varying hydrophobicity and net charges and evaluated their cell permeability, mitochondrial localization and toxicity. The overall increase in hydrophobicity had insignificant effect in mitochondrial localization while maintaining high cell permeability. Moreover, we concluded that a certain degree of a positive net charge was critical for mitochondrial localization. Our novel mitochondria-targeting peptoids present a highly selective and robust delivery system for bioactive molecules.

Poster Presentation : **LIFE.P-306**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Backbone Dynamics of Thermophile single-stranded binding protein from Sulfolobus solfataricus at room temperature and high temperature

Min June Yang, Chin-ju Park[1,*]

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

Single-stranded DNA (ssDNA) binding proteins (SSB) are necessary for the DNA replication, recombination, and repair process of all organisms. Most organisms overexpress their SSBs in high-stress conditions. Hyperthermophilic archaea Sulfolobus solfataricus (S. solfataricus), overexpresses its SSB (S. solfataricus SSB (SsoSSB)) for protecting ssDNA during DNA metabolisms. Most structural studies regarding SsoSSB have been performed at room temperatures, such as the crystal structure of apo SsoSSB and its ssDNA-bound form determined by NMR spectroscopy were reported. In order to understand how SsoSSB maintains its structure even at high temperatures, multidimensional NMR experiments were performed for SsoSSB at 298K and 323K. Relaxation parameters such as T1, T2, and hetNOE were collected to understand dynamic behavior of the protein. We figured out SsoSSB is ordered even at 323K and has a similar fold as 298K. The beta wing (between beta 2 and 3) region, which is expected to be important for DNA binding, was predicted to be flexible at both room and high temperatures. Our NMR study provide an understanding of the dynamic features of thermophile proteins.

Poster Presentation : **LIFE.P-307**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

A Simple Protein Histidine Kinase Activity Assay for High-throughput Inhibitor Screening

Su min Choi, Shin Hyeon Lee, Jung-Min Kee[1,*]

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

Two-component systems of bacteria play many crucial roles in antibiotic resistance, virulence, and biofilm regulation. Accordingly, TCS inhibitors have been investigated as attractive antibacterial drug candidates. Current HK activity assays are hindered by the notorious instability of the phosphohistidine (pHis) product. To overcome these difficulties, we developed a simple and high-throughput screening method named **AUDECY** (**AU**tophosphorylation-**DE**phosphorylation **CY**cle assay). This convenient kinetic assay successfully measured the enzyme activity of multiple HKs, especially those with very low pHis levels, thereby overcoming the limitation of current endpoint HK assays. Through a high-throughput screening with this method, we also identified a potent VanS HK inhibitor, which sensitized vancomycin-resistant *Enterococcus faecium* (VRE) toward vancomycin, highlighting the potential of this assay in HK inhibitor discovery.

Poster Presentation : **LIFE.P-308**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Discovery of PHPT1 inhibitors and elucidation of inhibition mechanism

Hyeong Jun Kim, Hoyoung Jung, Jung-Min Kee*

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

Histidine phosphorylation is one of the less-explored post-translational modifications (PTMs) because of its instability, but this modification is crucial to signal transduction and cell metabolism. Phosphohistidine phosphatase 1 (PHPT1) is a mammalian phosphatase specific to phosphohistidine (pHis) residues, and it plays a key role in cytoskeletal reorganization and cancer cell proliferation. In addition, its activity has made it challenging to isolate and detect pHis-harboring proteins in biological samples. Due to its unique catalytic mechanism, PHPT1 is insensitive to general phosphatase inhibitors, and no PHPT1-specific inhibitor has been reported. Here, we describe the first covalent inhibitor of PHPT1, discovered by high throughput screening. Using LC-MS/MS and mutational studies, we also identified the inhibitor-binding residue, laying foundations for further development of other covalent PHPT1 inhibitors. Our inhibitors are expected to facilitate further pHis studies by preserving the pHis through PHPT1 inactivation.

Poster Presentation : **LIFE.P-309**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Analysis of differentially expressed genes using RNA-Seq data of long-tailed chickens

Yunjeong Noh, Han-ha Chai*

National institute of animal science, Rural Development Administration, Korea

Renewing of plumage or molting is a critical stage in the life cycle of birds. During the molting period, the reproductive system of birds undergoes morphological and functional tissue remodeling. The present study investigated the effect of molt on gene expression in blood samples of Ginkkoridak, a Korean long-tailed chicken. RNA-sequence analysis was carried out using blood samples of 10 chickens before and after molting. The gene expression level using RNA-Seq transcriptome data was checked for differentially expressed genes through pairwise comparison using the cuffdiff program. Based on the absolute value log2 fold change >1 and P-value

Poster Presentation : **LIFE.P-310**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis of A/T Specific DNA Stains with Enhanced Optical Properties

Jaeyoung Bae, Kyubong Jo[*]

Department of Chemistry, Sogang University, Korea

Single-molecule imaging of large DNA is a powerful tool for DNA analysis. Sequence-specific DNA stains can derive sequence information from fluorescence microscope images. In the previous study, we reported a novel DNA stain, TAMRA-linked polypyrrole that specifically binds to adenine and thymine base pairs. Furthermore, TAMRA-polypyrrole showed no fluorophore-mediated photocleavage and structural deformation, common undesirable features of organic DNA stains. However, the low brightness and photostability of TAMRA limited its usage. Thus, we substituted TAMRA with other fluorophores: SiR, sfGFP, Alexa Fluor 647, and Atto 647N. Among them, Atto 647N-linked polypyrrole showed the best optical properties. In addition, we tried to identify genomic DNA fragments from E.coli by aligning them with in silico A/T frequency map. However, sole use of A/T specific DNA stain was not sufficient to identify the DNA fragments. Thus, we adopted another sequence-specific DNA label for additional verification. Direct Labeling Enzyme 1 introduces fluorophores at CTTAAG sequence without DNA breakage. By combining A/T specific DNA stain and sequence-specific labeling, we tried to make a genome map of E.coli.

Poster Presentation : **LIFE.P-311**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fluorometric detection of SARS-CoV-2 variantsusing ligation-coupled rolling circle amplification of viral RNA

Jamin Ku, Dong-Eun Kim*

Department of Bioscience & Biotechnology, Konkuk University, Korea

Since SARS-CoV-2 variant was first discovered in the UK in September 2020, many variants have emerged all over the world. Most of major variants such as alpha and delta variants have mutations in the spike protein of SARS-CoV-2. The mutant virus infects faster than wild-type virus and degrades the effectiveness of existing vaccines. Therefore, rapid and exact diagnosis of SARS-CoV-2 variants is needed for assessment of COVID-19 pandemic. We developed a fluorometric method for detection of SARS-CoV-2 variants by combining ligation and Rolling Circle Amplification (RCA) of viral RNA. In the presence of wild-type SARS-CoV-2 RNA, there is no ligation of the padlock DNA, which is annealed to corresponding viral RNA, due to single nucleotide mismatch at the terminal between linear padlock DNA and target RNA. On the other hand, in the presence of SARS-CoV-2 variant that has single nucleotide polymorphism (SNP), ligation of padlock DNA occurs by splint R ligase because of the linear padlock DNA and target RNA. The ligated circular padlock DNA is then used for the subsequent RCA reaction, in which isothermal viral RNA amplification is accomplished with production of long stretched single-stranded DNA containing G-quadruplex. Fluorophore thioflavin T is then intercalated into the G-quadruplex with enhanced green fluorescence. Through this isothermal viral RNA amplification combined with SNP-discerning ligation, we can identify presence of SARS-CoV-2 variants by fluorescence detection. Our fluorometric detection using ligation-coupled RCA method would be useful for sensitive and accurate diagnosis of SARS-CoV-2 variants with SNP.

Poster Presentation : **LIFE.P-312**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fluorometric detection of SARS-CoV-2 viral RNA using tandem isothermal gene amplification

Hyojin Lee, Yong-Joo Jeong[1], Dong-Eun Kim*

Department of Biotechnology, Konkuk University, Korea
[1]*Department of Applied Chemistry, Kookmin University, Korea*

Detection of SARS-CoV-2 through fast, accurate, and sensitive testing is the most important and fundamental step to cope with COVID-19 epidemic. We developed a sensitive fluorometric assay for detecting SARS-CoV-2 viral RNA with PCR-free method. This assay system based on tandem isothermal gene amplification is composed of ternary Rolling Circle Amplification (t-RCA) and subsequent strand displacement amplification coupled with RCA (SDA-RCA). In t-RCA, viral RNA forms a ternary initiation complex with the hairpin primer and RCA circular template. The t-RCA product, which contains multiple-repeated dumbbell-like structures, participate in the SDA reaction. The SDA reaction produces large amounts of short single-stranded DNAs (ssDNAs), which act as primers for the second RCA reaction. A long stretch of ssDNA containing repeated copies of the G-quadruplex was produced in the second RCA. Subsequently, fluorometric detection of amplified viral gene was accomplished by monitoring emission of strong fluorescence by thioflavin T that intercalates into the G-quadruplex. Fluorometric analysis enabled sensitive detection of SARS-CoV-2 RNA as low as 1.8 pM with a linear range between 2 pM and 10 nM within 1 h. Hence, this novel method for direct detection of viral RNA via tandem gene amplification can be useful to diagnose COVID-19 and other viral infection with high sensitivity and accuracy.

Poster Presentation : **LIFE.P-313**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Uncovering different roles of two acinetobactin isomers in fighting against nutritional immunity

Mingi Kim, Hak Joong Kim[1,*], Do Young Kim[2]

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

The antibiotic resistance of *Acinetobacter baumannii* has emerged as a serious concern because of the continuing paucity of effective treatment options. During *A. baumannii* infection, cellular machineries associated with acquisition of essential nutrients such as iron are known to act as significant virulence factors. One of such machineries is the siderophore biosynthesis and uptake system, in charge of scavenging iron against nutritional immunity that creates iron deficiency at the infection sites. Siderophores are small molecule metabolites that bacteria utilize to uptake Fe(III) intracellularly via the cognate transporters. *A. baumannii* produces three different siderophores, among which acinetobactin plays a major role in iron supply. With respect to the structure of acinetobactin, two isomeric forms, possessing either oxazoline (Oxa) or isoxazolidinone (Isox) at the respective core, were identified, but the difference in their function under physiological conditions was not fully elucidated. This poster describes our recent findings addressing this issue. Specifically, growth promotion assays clearly revealed that Oxa exhibits higher iron delivery activity than Isox, and it is the only isomer making interactions with the acinetobactin uptake machinery. In addition, Oxa was found to constitute a strong iron complex whose iron cannot be displaced by Isox. Finally, both acinetobactins were able to scavenge iron from the host iron-sequestering proteins. These results led us to propose a new model of acinetobactin-based iron acquisition by *A. baumannii* at infection sites, in which Oxa acts as the principal siderophore, whereas Isox plays a minor role in iron supply.

Poster Presentation : **LIFE.P-314**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

Spliceosomal recycling factor Sart3 RRM recognition of U6 snRNA investigated by NMR

Kyeong-Mi Bang, Ji-Yeon Shin, Hyun Kyu Song[1], Jeong-Yong Suh[2], Nak-Kyoon Kim*

Advanced Analysis Center, Korea Institute of Science and Technology, Korea
[1]*Division of Life Sciences, Korea University, Korea*
[2]*Department of Agricultural Biotechnology, Seoul National University, Korea*

Spliceosome is a large and dynamic RNA-protein complex, which is made up of five small nuclear ribonucleoproteins (U1, U2, U4, U5, and U6 snRNPs). In the splicing process, the components of spliceosome are recycled for a new round of catalysis. Among many recycling factors, squamous cell carcinoma antigen recognized by T-cells 3 (SART3) is required to adopt the U6 snRNA for the formation of the U4/U6 snRNP complex in human. SART3 consists of a 12 half-a-tetratricopeptide (HAT) repeat domains in N-terminal, a nuclear localization signal (NLS) sequence, two RNA recognition motifs (RRMs), and an extension of 10 highly conserved amino acids in C-terminal (C10). Among these domains, the RRM domains are suggested to be involved in the binding of the U6 snRNA. U6 snRNA is believed to play an essential role in the catalytic mechanism of pre-mRNA splicing. I designed several constructs of U6 snRNA containing a asymmetric bulge, which are predicted to interact with RRMs of SART3. Above all, I investigated the tertiary interaction between RRMs and U6 snRNA using electrophoretic mobility shift assay (EMSA). I found that the asymmetric bulge of U6 snRNA interacts with SART3 and if there is a stem region around the asymmetric bulge, it binds better with SART3. In addition, I confirmed that SART3 binds better with U6 snRNA in the dimer with four RRMs than in the monomer with two RRMs. And then, I measured binding affinity between SART3 and U6 snRNAs using isothermal titration calorimetry (ITC). Also, I performed a structural investigation of the tertiary interaction between RRM1 and RRM2 and asymmetric bulge of U6 snRNA (U6 33-54) using NMR spectroscopy, and also determined the tertiary structure of RRM1 and RRM2 and the residues interaction with U6 snRNA. These results will provide a structural basis for the complex formation of U4/U6 snRNP mediated by SART3.

Poster Presentation : **LIFE.P-315**
Life Chemistry
Exhibition Hall 1 THU 11:00~12:30

NMR study of ligand & metal dependent riboswitch folding

Ji-Yeon Shin, Kyeong-Mi Bang, Hyun Kyu Song[1], Nak-Kyoon Kim[2,*]

Advanced analysis center, Korea Institute of Science and Technology, Korea
[1]*Division of Life Sciences, Korea University, Korea*
[2]*Advanced Analysis Center, Korea Institute of Science and Technology, Korea*

Riboswitch is a structural RNA motif that is located at the 5'- end of bacterial mRNA, regulating protein expression upon binding small molecules. Riboswitch is composed of aptamer domain and expression platform. The aptamer domain specifically binds a ligand, and the expression platform is responsible for the gene expression via switching its conformation between two different secondary structures in response to ligand binding. I have studied the structural folding of cyclic-di-GMP (bis-(3′-5′)-cyclic dimeric guanosine monophosphate, c-di-GMP) riboswitch using NMR spectroscopy. Cyclic-di-GMP is widely used by bacteria to regulate processes ranging from biofilm formation to the expression of virulence genes. Cyclic-di-GMP riboswitch is the first known example of a gene-regulatory RNA that binds a second messenger, and it is present in pathogens such as *Clostridium difficile, Vibrio cholerae and Bacillus anthracis*. The secondary structures of apo- and holo- state riboswitch were determined through assignment of 2D ^{1}H-^{1}H NOESY and ^{1}H-^{15}N HSQC spectra. I have observed the chemical shift changes as well as the appearance of the new resonances in ^{1}H-^{15}N HSQC spectra upon addition of Mg^{2+} ions and c-di-GMP to RNA, indicating that the conformational changes of the riboswitch and new base-pair formation. Furthermore, HNN-COSY identified several reverse Hoogsteen AU basepairs and a non-canonical GA basepair. I also performed NMR and ITC analysis with site-specific mutants disrupting tertiary interactions known to play an important role in RNA folding. I confirmed that these tertiary interactions serve to pre-organize the aptamer domain of riboswitch. Through acurate analysis of NMR and ITC data, detailed metal and ligand dependent base-pair formation and conformational changes of RNA were identified.

Poster Presentation : **ORGN.P-294**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Terpyridine-Strapped Calix[4]pyrrole: An Ion Pair Receptor for the Recognition of Lithium Chloride

Nam Jung Heo, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A calix[4]pyrrole strapped with a terpyridine via ester linkage was synthesized as an ion pair receptor. ^{1}H NMR spectroscopic analyses revealed that the receptor was able to bind LiCl with remarkably high affinity. In 10% methanol in chloroform, the receptor was found to bind chloride in the presence of the lithium cation forming the LiCl complex. By contrast, without Li$^+$ existing in the solution, no evidence for chloride binding was found. For the LiCl complex of the receptor, the lithium cation was complexed with the terpyridine moiety while the chloride anion was hydrogen bonded to the NHs of the calix[4]pyrrole. These experimental findings were supported by single X-ray crystal diffraction analysis.

Poster Presentation : **ORGN.P-295**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Calix[4]pyrrole biscrowns having a deep cavity and their ion pair recognition properties

Juho Yang, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

Calix[4]pyrrole bis-crown-n (n = 3, 4, and 5) having deep cavities have been synthesized as ion pair receptors. It was revealed by ^{1}H NMR spectroscopic analysis and single crystal X-ray diffraction analyses that the ion receptors were able to bind cesium salts highly selectively over other alkali metal halide salts. In these cases, the cesium cation was bound to the crown ether moieties with the halide anions being hydrogen bonded to the calix[4]pyrrole NHs. By contrast, when non-coordinating perchlorate anion was used as the counter anion to the alkali metal cations, only the Na+ cation was found to be complexed the receptors with 1:1 stoichiometry. Upon addition of fluoride or chloride to the solutions of the receptors in the presence of Na^+ and Cs^+, respectively, ion pair complexes were formed within the receptors for Cs^+ while de-complexation took place for Na^+.

Poster Presentation : **ORGN.P-296**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Calix[4]pyrrole with extended indole as highly selective receptor for the phosphate anion

Ju hyun Oh, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A new calix[4]pyrrole-based anion receptor having two diagonal amido indoles has been synthesized. It was proved by ^{1}H NMR spectroscopic analyses and UV/vis spectroscopic analyses that the receptor possesses an ability to recognize with high affinity oxo-anions including $H_2PO_4^-$ and $HP_2O_7^{3-}$ (as their tetrabutylammonium salts) as well as spherical halide anions in chloroform with the highest preference for the dihydrogen phosphate anion ($K_a > 10^4$). Different binding modes of the receptor for halides and the oxo-anions were revealed via ^{1}H NMR spectroscopic and single crystal X-ray diffraction analysis. Specifically, the receptor forms hydrogen bonds with the dihydrogen phosphate anion via the indole NHs and amide NHs as well as two pyrrolic NHs of the calix[4]pyrrole framework. In this case, the calix[4]pyrrole unit adopted the unprecedent 1,3-alternate conformation. The carbonyl oxygen atoms of the ethyl ester groups were also found to take part in the anion binding via hydrogen bond. By contrast, for halide anions, indole and pyrrolic NHs but not amide NHs took part in recognition of these anions with the calix[4]pyrrole unit locked in cone conformation.

Poster Presentation : **ORGN.P-297**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Dipyrrolic-N-aryl-Naphalimide as Building blocks for Construction of Macrocyclic Aromatic Compounds and Their Anion Binding Features

Jaehyeon Kim, Sung Kuk Kim[*]

Department of Chemistry, Gyeongsang National University, Korea

We have successfully prepared dipyrrolic-N-aryl-naphthalimide **1** and dipyrrolic naphthalene **2** as anion receptors as well as building blocks for synthesis of new macrocyclic anion receptors and aromatic compounds as a new member of expanded porphyrin family. It was revealed by ^{1}H NMR and fluorescence spectroscopic analyses that receptors **1** and **2** were able to bind anions such as fluoride, chloride, and oxo-anions including dihydrogen phosphate, sulfate, and pyrophosphate. Upon addition of anions to the acetonitrile solutions of receptors **1** and **2**, large downfield shift of the proton signals corresponding to pyrrolic NHs and naphthalic aromatic CHs in ^{1}H NMR spectra suggested that both NHs and CHs participate in anion binding via hydrogen bonds.

Poster Presentation : **ORGN.P-298**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

A Calix[4]pyrrole-Based Fluorescent Sensor for Trinitroaromatic Explosives

Areum Lee, Sung Kuk Kim*

Department of Chemistry, Gyeongsang National University, Korea

A calix[4]pyrrole-based fluorescent sensor **1** diametrically bearing electron-donating pyrene groups was synthesized for sensing of trinitroaromatic explosives (TNB and TNT). It was revealed by ^{1}H NMR and fluorescence spectroscopic analysis that receptor **1** has ability to recognize TNT and TNB in chloroform via hydrogen bonding interactions between the nitro groups of the explosives and the pyrrolic and amide NHs of the receptor. In addition, the facing pyrene groups of the receptor were found to form charge transfer complex with the electron-deficient TNT and TNB accompanying colour changes and fluorescence quenching.

Poster Presentation : **ORGN.P-299**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Calix[4]arene tetra-Indole-2-Carboxamide: An Ion-pair Receptor for the Recognition of Lithium Chloride

Sung Kuk Kim*, Seung Hyeon Kim

Department of Chemistry, Gyeongsang National University, Korea

A new calix[4]arene bearing four indole-2-carboxamide substituents 1 on the upper rim has been prepared as an ion pair receptor. The binding ability of the receptor for halogen anions and various alkali metal halide salts was tested in organic media (CDCl3 and DMSO-d¬6¬, v/v, 9:1) by monitoring the changes in their 1H NMR spectra as a function of added anion and/or cation. The resulting spectral changes proved that the receptor binds lithium halide salts selectively over other alkali metal halide salts. It was also found that the pre-bound lithium cation within receptor facilitated anion binding to the receptor or vice versa. Single crystal X-ray diffraction analyses of the LiCl complex of the receptor revealed that LiCl is complexed within the receptor as a contact ion pair. The chloride anion was also hydrogen bonded to the indole NHs while the lithium cation is coordinated the carbonyl oxygen atoms of the amide groups. On the basis of the present findings, we propose that incorporation of four indole-2-carboxamide units within an overall calix[4]arene-based recognition framework could produce a preorganized receptor system that displays modest preference for LiCl.

Poster Presentation : **ORGN.P-300**

Organic Chemistry

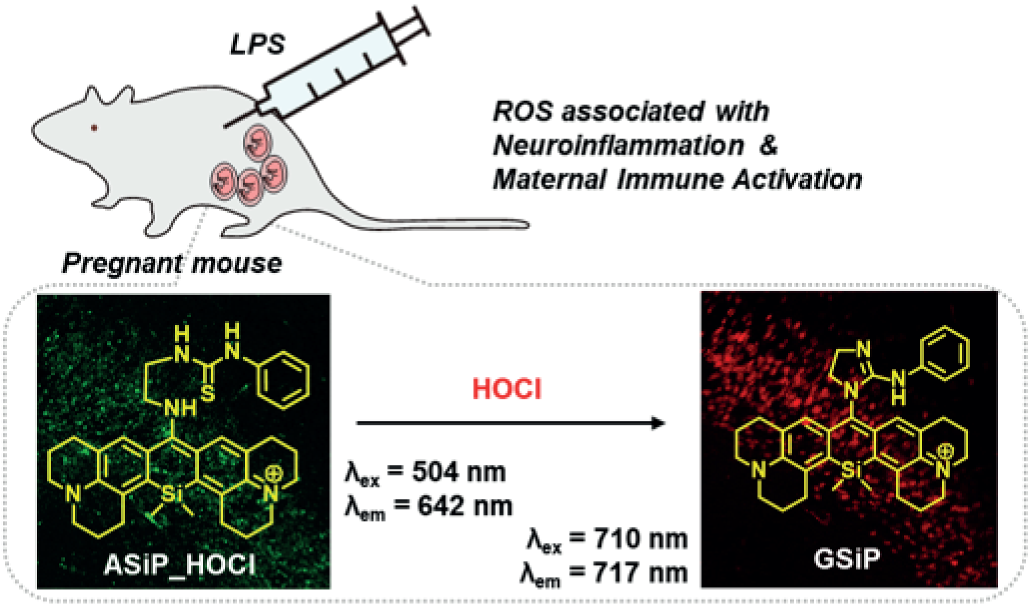
Exhibition Hall 1 FRI 11:00~12:30

Ratiometric Detection of Hypochlorous Acid in Brain Tissues of Neuroinflammation and Maternal Immune Activation Models with a Deep-Red/Near-Infrared Emitting Probe

Kyeong Hwan Kim, **Kyo Han Ahn**[1,*]

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

Reactive oxygen species (ROS) produced by inflammatory response in the brain are associated with various neurological disorders. To investigate ROS-associated neuroinflammatory diseases, fluorescent probes with practicality are in demand. We have investigated hypochlorous acid, an important ROS, in the brain tissues of neuroinflammation and maternal immune activation (MIA) model mice, using a new fluorescent probe. The probe has outperforming features over many known probes, such as providing two bright ratio signals in cells and tissues in deep-red/near-infrared wavelength regions with a large spectral separation, in addition to being strongly fluorescent, photo- and chemo-stable, highly selective and sensitive, fast responding, and biocompatible.We have found that the level of hypochlorous acid in the brain tissue of a neuroinflammatory mouse model was higher (2.7−4.0-fold) compared with that in normal brain tissue. Furthermore, the level of hypochlorous acid in the brain tissue of a MIA mouse model was higher (1.2−1.3-fold) compared with that in the normal brain tissue. The ‘robust’ probe provides a practical tool for studying the ROS-associated neurological disorders.


LPS
ROS associated with
Neuroinflammation &
Maternal Immune Activation
Pregnant mouse
ASiP_HOCl
HOCl
λex = 504 nm
λem = 642 nm
λex = 710 nm
λem = 717 nm
GSiP

Poster Presentation : **ORGN.P-301**

Organic Chemistry

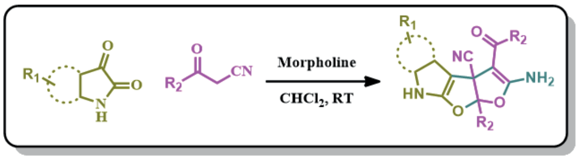
Exhibition Hall 1 FRI 11:00~12:30

Direct Access of Dihydrofuro [3',2':4,5]furo[2,3-b]indole via Isatine and 2-Cyanoacetophenone

Maruti Yadav, Yeon Tae Jeong*, Hoon Heo, Byung-Gwon Cho

Department of Display Engineering, Pukyong National University, Korea

A series of novel transformation of Dihydrofuro [3', 2’:4,5]furo[2,3-b]indole with Isatine and α-cyanoketones have been achieved for the first time. Delivering a series of skeletally thoroughly different Dihydrofuro [3',2':4,5]furo[2,3-b]indole derivatives. A range of novel transformations of the products can be realized. This synthetic protocol could be applicable to a wide range of substrates. The desired products are easily separated and purified by simple crystallization.



Poster Presentation : **ORGN.P-302**

Organic Chemistry

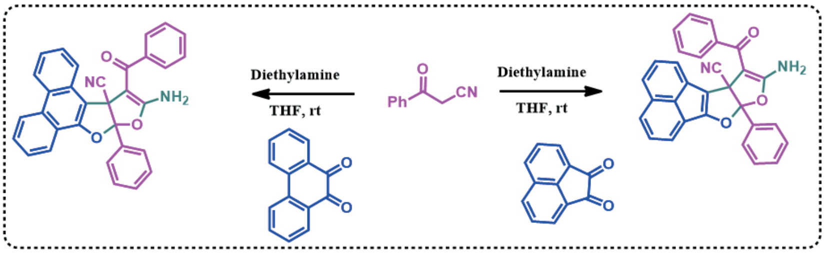
Exhibition Hall 1 FRI 11:00~12:30

Catalyst Based Divergent Reaction of Benzoylacetonitrile with acenaphthylene-1, 2-Dione: Access to Spiro-dihydrofurofuran and dihydrofurofuran Derivatives.

Maruti Yadav, Yeon Tae Jeong*, Hoon Heo, Byung-Gwon Cho

Department of Display Engineering, Pukyong National University, Korea

A simple and efficient synthetic protocol for the syntheses of spiro dihydroacenaphtho[1,2-b]furo[3,2-d]furan and dihydrofuro[2,3-b]phenanthro[9,10-d]furan derivatives via a one pot three-component reaction catalyzed by organo-based catalyst has been successfully developed under the different reaction condition. The reactions afforded spiro dihydroacenaphtho [1, 2-b] furo [3, 2-d] furan in good to excellent yields. While phenanthrene-9, 10-dione were used in reaction, a product scaffold of dihydrofuro [2, 3-b] phenanthro [9, 10-d] furan was obtained in moderate to good yields.



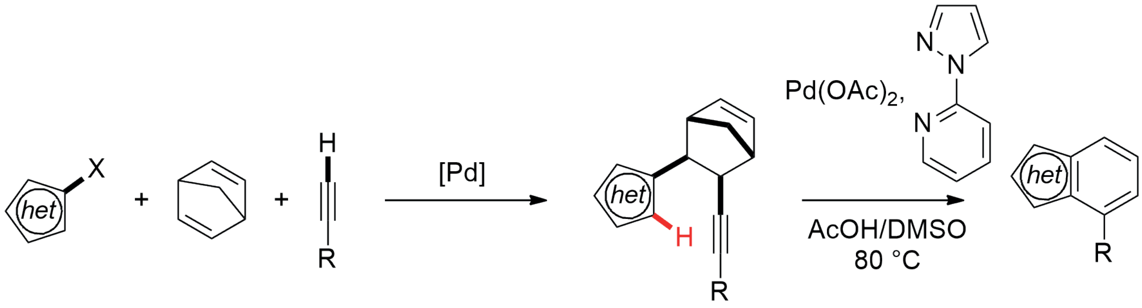
Poster Presentation : **ORGN.P-303**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Pd-Catalyzed Cyclization of Alkynyl Norbornene Derivatives for the Synthesis of Benzofused Heteroarenes

Hayeon Kwak, Jung Min Joo*

Department of Chemistry and Chemistry Institute for Functional Materials, Pusan National University, Korea

Benzo-fused heteroarenes are important structures that are commonly found in pharmaceuticals and natural products. Traditionally, cyclization reactions of alkyne-tethered heteroarenes have been performed using Au and Ag catalysts to afford benzofused heteroarenes. However, it is challenging to prepare cyclization precursors for these reactions because of requiring several steps. We developed a new method for the cyclization of heteroarenes tethered with alkynes through a norbornene bridge using Pd catalyst and acetic acid. The precursors were readily prepared by a three-component coupling reaction of heteroaryl halides, norbornadiene, and terminal alkynes. With $Pd(OAc)_2$, 2-(pyrazol-1-yl)pyridine, and acetic acid, the cyclization was achieved to provide a variety of benzofused heteroarenes including (di)benzothiophene, indazole, indole, carbazole, and benzofuran, with aryl and alkyl substituents at the C4(C7) position. In the cyclization process, the norbornene served as a two-carbon building block through retro-Diels–Alder reactions while promoting the cyclization by putting the heteroarene and alkyne in proximity. This approach will allow the rapid synthesis of substituted benzofused heteroarenes in high yields.



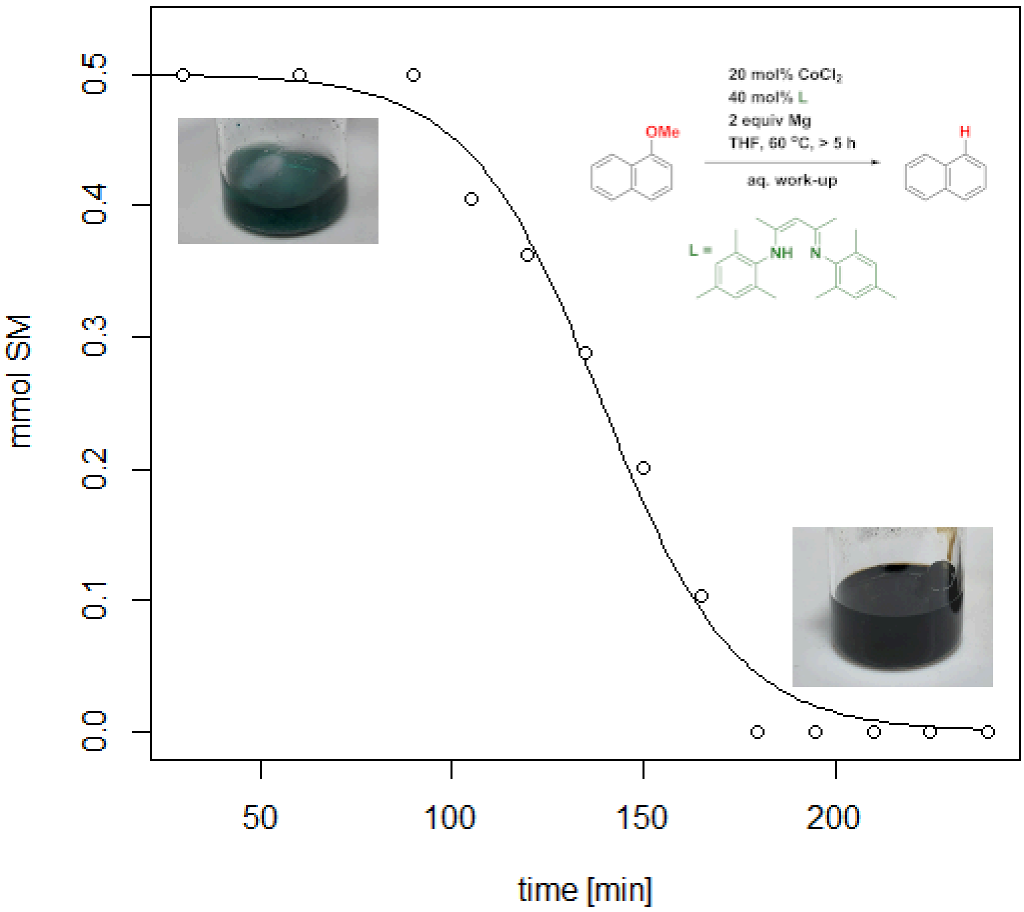
Poster Presentation : **ORGN.P-304**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mechanistic Study of Cobalt-Catalysed C-O Bond Activation

Ewa Pietrasiak, Eunsung Lee[1,*]

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

Aryl ethers are an attractive alternative for aryl halides in cross-coupling reactions due to good availability, lack of halogenated waste, and atom economy.[1] Most examples of C-O bond cleavage in aryl ethers reported to date involve homogeneous nickel catalysis.[2] In our laboratory, we demonstrated that this transformation can be achieved with a cobalt catalyst, previously applied for C-F bond activation.[3,4] Hence, in presence of cobalt(II) chloride, magnesium, and a nacnac-type ligand C-O bond activation followed by borylation could be accomplished. Herein, we present mechanistic studies of the C-O activation step in 1-methoxynaphthalene as a model substrate. We found that under standard conditions the reaction exhibits an induction period of ~1-2 h, followed by rapid consumption of the starting material. The length of the induction period correlates with the appearance of a black precipitate we denoted as “cobalt black”. In addition, the conversion decreases at higher catalyst loading or in the presence of mercury. Based on these observations, we postulate that the “cobalt black” acts as a heterogeneous catalyst for the C-O bond cleavage reaction.[5,6]1.D. G. Yu, S. Luo, F. Zhao, Z. J. Shi, Homogeneous Transition-Metal-Catalyzed C-O Bond Activation, Wiley Blackwell, 2014.2.M. Tobisu, N. Chatani, Acc. Chem. Res. 2015, 48, 1717–1726.3.S. Lim, H. Cho, J. Jeong, M. Jang, H. Kim, S. H. Cho, E. Lee, Org. Lett. 2020, 7387–7392.4.S. Lim, D. Song, S. Jeon, Y. Kim, H. Kim, S. Lee, H. Cho, B. C. Lee, S. E. Kim, K. Kim, et al., Org. Lett. 2018, 20, 7249–7252.5.J. A. Widegren, R. G. Finke, J. Mol. Catal. A Chem. 2003, 198, 317–341.6.J. G. De Vries, Dalt. Trans. 2006, 421–429.


mmol SM
0.0
0.1
0.2
0.3
0.4
0.5
50
100
150
200
time [min]
OMe
20 mol% $CoCl_2$
40 mol% L
2 equiv Mg
THF, 60 °C, > 5 h
aq. work-up
H
L =
NH
N

Poster Presentation : **ORGN.P-305**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Skullcapflavone II, a polymethoxylated flavone isolated from Scutellaria baicalensis

Jisu Yoo, Sangku Lee[1,*]

Chungbuk Natioanl University, Korea
[1]*KRIBB, Korea*

Skullcapflavone II (SFII; 5,2'-dihydroxy-6,7,8,6'-tetramethoxy flavone), isolated from the roots of Scutellaria baicalensis, showed potent anti-inflammatory, hepatoprotective, antioxidant, and anticancer activities. Despite its various pharmacological activities, the synthesis of skullcapflavone II is not reported yet. We wish to present the synthesis of SFII.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **ORGN.P-306**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Rhodamine based fluorescent probe as acid sensor

Jinsung Tae[*], Yoon Jeong Lee

Department of Chemistry, Yonsei University, Korea

Chemosensor has been widely used to detect the target molecules through chemical reactions. Rhodamine is an ideal model to construct chemosensor because of it's outstanding brightness, solubility and photostability. For these reasons, Rhodamine based fluorescent chemosensor have been used for proton detection in aqueous solution. In biological systems, pH plays a central role in many cellular events such as cell growth, cell adhesion and other cellular process. The rhodamine 6-membered amide is converted from spiro-cyclic form to open form by protonation of the electron donating site. In conclusion, this rhodamine structure showed highly sensitive to proton in aqueous media.

Poster Presentation : **ORGN.P-307**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Linear-Shaped High-Efficiency Thermally Activated Delayed Fluorescence Emitters with Deep-Blue Color Coordinates

Youngnam Lee, Jong-in Hong*

Division of Chemistry, Seoul National University, Korea

Highly efficient 10-(5,9-dioxa-13*b*-boranaphtho[3,2,1-de]anthracen-7-yl)-10*H*-dispiro[acridine-9,9′-anthracene-10′,9″-fluorene] (OBOtSAc) and 10-(2,12-di-*tert*-butyl-5,9-dioxa-13*b*-boranaphtho[3,2,1-de]anthracen-7-yl)-10*H*-dispiro[acridine-9,9′-anthracene-10′,9″-fluorene] (tBuOBOtSAc) emitters, comprising almost perpendicularly linked rigid 5,9-dioxa-13*b*-boranaphtho[3,2,1-de]anthracene (OBO) electron acceptors and a rigid and linear tri-spiral acridine electron donor, are reported here. OBOtSAc and tBuOBOtSAc show deep-blue emission (λ_{max} = 452 and 446 nm) with narrow full width at half maximum (FWHM) values of 50 and 48 nm, respectively. Due to the rigid and twisted structures, and the appropriate singlet and triplet energy levels of both emitters, 10 wt% doped films of OBOtSAc and tBuOBOtSAc in a bis[2-(diphenylphosphino)phenyl]ether oxide (DPEPO) host show efficient thermally activated delayed fluorescence (TADF) emission and photoluminescence quantum yields (PLQYs) of 97% and 90%, respectively. Moreover, linear-shaped OBOtSAc and tBuOBOtSAc lead to excellent horizontal emitting dipole orientations (88% and 90%, respectively). Consequently, organic light-emitting diode (OLED) devices using OBOtSAc and tBuOBOtSAc exhibit maximum external quantum efficiencies (EQEs) of 31.2% and 28.2%, respectively, and Commission Internationale de l'Éclairage (CIE) coordinates of (0.147, 0.092) and (0.149, 0.061), respectively.

Poster Presentation : **ORGN.P-308**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Practical Synthesis of Norbixin and Its Ethyl Ester using Bromoacetate and Julia−Kocienski Olefination Protocol

Aleksei Golikov, Sangho Koo*

Department of Chemistry, Myongji University, Korea

Norbixin 1 and norbixin ethyl ester 2 were efficiently produced with 35% and 36% overall yield respectively. Practical synthesis of norbixin 1 had done by coupling of ethyl bromoacetate with C20 dialdehyde 6 and subsequent double elimination of the protected hydroxyl groups and bromine atoms of the coupling bromohydrin product. Norbixin ethyl ester 2 was synthesized by Julia−Kocienski olefination of a novel C7 benzothiazolyl-sulfone 11 and C10 2,7-dimethyl-2,4,6-octatrienedial 12

Poster Presentation : **ORGN.P-309**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Heterocycle Compounds Generation by using Mn(III)/Co(II)Catalyzed Oxidative Deacetylation

Yifan Zheng, Sangho Koo[1,*]

Department of Chemistry, Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

Efficient synthetic method for medicinally and opto-electronically important bichalcophenes is reported, which highlights Mn(OAc)3/CoCl2-catalyzed oxidative deacetylation of 1,5-dicarbonyl compounds that were easily prepared by conjugate addition of ethyl acetoacetate to,□α, β-unsaturated carbonyl compounds containing a chalcophene unit. Paal–Knorr reaction of the resulting 1,4-dicarbonyl compounds produced 4-phenyl-2,2′-bichalcophenes and their azaanalogues.The Manganese-mediated deacetylation reaction explored in this thesis can convert 1, 5- dicarbonyl compounds into 1, 4-dicarbonyl compounds (the substrate of Paal-Knorr reaction) at room temperature under the catalytic condition with the assistance of cobalt chloride. By combining this reaction with the classical five-element heterocyclic synthesis method Paal- Knorr reaction, heterocyclic compounds containing various functional groups and even oligoaromatic compounds can be generate easily.

Poster Presentation : **ORGN.P-310**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Study on the Synthesis of Phytofluene Using Julia-Koicenski Olefination and Wittig reaction

Hyein Kim, Chanyoung Boo, Sangho Koo*

Department of Chemistry, Myongji University, Korea

An efficient synthetic method of natural white carotenoids phytofluene has been developed by Julia-Koicenski Olefination and Wittig reaction start from farnesol. Unlike many natural carotenoids, phytofluene has an asymmetric structure in which one half side has one more double bond than the other half. In this study, synthesis was devised in a different direction from when synthesizing symmetric carotenoids. Farnesol derivative was coupled with C5-protected aldehyde by Wittig reaction, then the resulting deprotected C20-aldehyde was coupled with geranylgeraniol derivatives by Julia-Koicenski Olefination. In this method, all coupling reaction were performed at -78℃, resulting in the synthesis of phytofluene with high stereoselectivity with 99% E-form.

Poster Presentation : **ORGN.P-311**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fast Assembly and High-Throughput Screening of Structure andAntioxidant Relationship of Carotenoids

Gaosheng Shi, Sangho Koo[1,*]

Department of Energy Science and Technology, Myungji University, Korea
[1]*Department of Chemistry, Myongji University, Korea*

C20 heptaenyl diphosphonate 4 was prepared for one-pot synthesis of carotenoids 1. Olefination with various aromatic aldehydes allowed fast assembly of the corresponding carotenoids. The SAR of carotenoids was investigated by high throughput screening of ABTS and DPPH assays and their hierarchical clustering analysis. Antioxidant activity of carotenoids increased with the number of electron-donating substituents. Carotene 1a with multiple electron-donating substituents was most proficient, which showed better radical scavenging activities than β-carotene and lycopene.

Poster Presentation : **ORGN.P-312**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mechanism and Governing Factors of the Sequential Photon-Electron-Photon Catalytic Borylation of Aryl Bromides

Dong Yeun Jeong, Eun Jin Cho[1], Youngmin You[2,*]

chemical engineering and material science, Ewha Womans University, Korea
[1]Department of Chemistry, Chung-Ang University, Korea
[2]Chemical Engineering and Materials Science, Ewha Womans University, Korea

Photoredox catalysis enables a variety of organic transformations under mild conditions. However, the scope of photoredox catalysis is limited principally by electrochemical potentials derived from single photon. Multiphoton redox catalysis can circumvent the limitation because it utilizes non-frontier molecular orbitals with large thermodynamic driving forces for electron transfer. In this study, we have developed the two-photon-redox catalytic borylation protocol and investigated its mechanism. We used donor-acceptor dyad organophotocatalysts where the donor and the acceptor are phenylindolocarbazole and phenylbenzothienopyrimidine-benzonitrile(benzene), respectively. Photoillumination (18 W, white light) of DMSO containing bromoarene, bis(pinacolato)diboron, 1 mol % catalyst, and DBU produced the desired pinacolatoborylarene in an 86% yield. The borylation is initiated by rapid quenching of the excited-state catalyst by DBU with a rate constant for electron transfer of 4.2×10^{7} M^{-1} s^{-1}, producing the radical anion of the catalyst. Our transient spectroscopic and spectroelectrochemical experiments point to the second photon absorption of the long-lived radical anion of the catalyst. The resulting doublet excited-state radical anion is sufficiently cathodic to reduce bromoarenes, as inferred from its excited-state oxidation potential (-2.25 V vs SCE) being more negative than reduction potentials of bromoarenes.

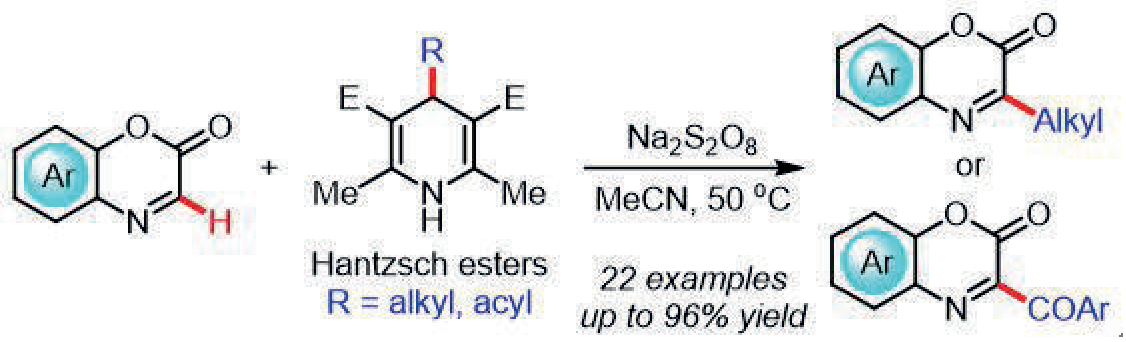
Poster Presentation : **ORGN.P-313**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Site-Selective Alkylation and Acylation of Benzoxazinones with 1,4-Dihydropyridines

Youjung Byun, In Su Kim[*]

College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea

The direct functionalization of N-heterocycles is a vital transformation for the development of pharmaceuticals, functional materials, and other chemical entities. Herein, the transition-metal-free alkylation and acylation of $C(sp^2)$–H bonds in biologically relevant 2-benzoxazinones with 1,4-dihydropyridines as readily accessible radical surrogates is described. Excellent functional group compatibility and a broad substrate scope were attained. Gram-scale reaction and transformations of the synthesized adducts via Suzuki coupling with heteroaryl boronic acids demonstrated the synthetic potential of the developed protocol.



Poster Presentation : **ORGN.P-314**

Organic Chemistry

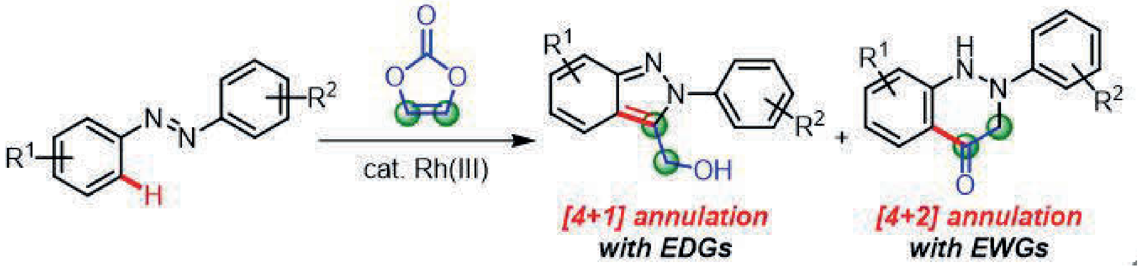
Exhibition Hall 1 FRI 11:00~12:30

Annulation of Azobenzenes using Vinylene Carbonate to Synthesize (2H)-Indazoles and Dihydrocinnolinones with Rh(III) Catalysis

Minseo Park, In Su Kim[*]

College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea

The Rh(III)-catalyzed C–H functionalization and subsequent intramolecular cyclization between azobenzenes and vinylene carbonate is described herein. Depending on the electronic property of azobenzenes, this transformation results in the formation of (*2H*)-indazoles or dihydrocinnolin-4-ones through the generation of *ortho*-alkylated azo-intermediates followed by decarboxylation. Surprisingly, vinylene carbonate acts as an acetaldehyde or acetyl surrogate to enable the [4+1] or [4+2] annulation reaction. This transformation is characterized by its mild reaction conditions, simplicity, and excellent functional group compatibility.



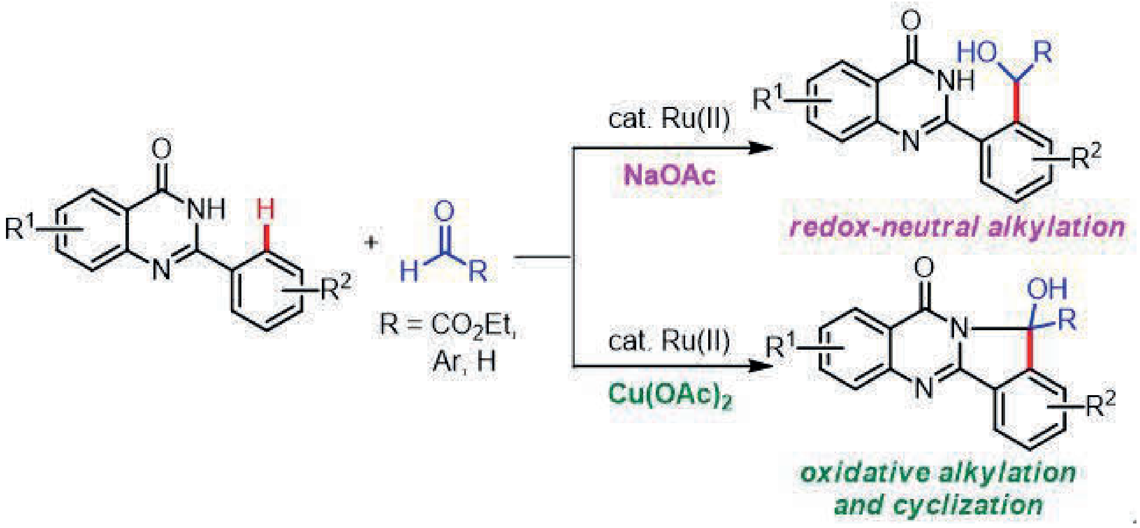
Poster Presentation : **ORGN.P-315**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

C-H Hydroxyalkylation and Oxidative cyclization of Quinazolinone moiety under Ruthenium(II) Catalyst

Junghyea Moon, In Su Kim*

College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea

Quinazolinone is the most interesting structure found in a great number of pharmaceutical ingredients and natural products. Especially, polycyclic quinazolinones such as rutaecarpine, synthetic AchE inhibitor and luotonins have lately attracted significant attention by merit of their interesting physical and biological properties. Consequently, the abundance of polycyclic quinazolinones in bioactive molecules has led to much effort for the development of efficient methods for their synthesis. Transition-metal-catalyzed C–H functionalization have been one of the most interesting topics because of environmental sustainability and atom/step economy in organic synthesis. In this context, much attention has been focused on the C(sp^2)–H addition with polar π-unsaturated compounds, such as aldehydes, imines, and isocyanates, leading to the efficient construction of carbocyclic and heterocyclic products. Significant progress in this direction has been realized by using ruthenium catalysts due to their high efficiency, and various functional group tolerance under mild reaction conditions. With essential structural features of unmasked 2-aryl quinazolin-4(*3H*)-ones with inherent directing group capability, we in this context report the Ru(II)-catalyzed C–H addition and oxidative cyclization of 2-aryl quinazolinones with aldehydes. Remarkably, the use of Cu(OAc)2 as an external oxidant demonstrate the synthetic potential for the direct formation of tetracyclic isoindoloquinazolinones.


R1
O
NH
H
N
R2
+
O
H
R
R = CO2Et, Ar, H
cat. Ru(II)
NaOAc
HO
R
redox-neutral alkylation
cat. Ru(II)
Cu(OAc)2
OH
oxidative alkylation and cyclization

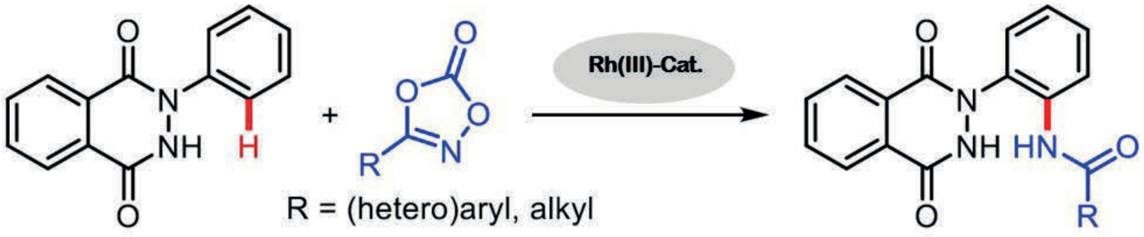
Poster Presentation : **ORGN.P-316**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

C-H Amidation of Phthalazinone with Dioxazolones under Rh(III)-Catalysis

Suho Kim, In Su Kim*

College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea

There are so many heterocycles in nature, containing nitrogen and closely related to heterocyclic medicinal applications. The phthalazinone skeleton is ubiquitous structural motif, which plays a central role in pharmaceutics; anti-inflammatory, anti-microbial, etc. Recently, the catalytic C−H amination has been used in the most ways for synthesis of the *N*-heterocyclic compounds. And currently, the new schematic method with phthalazinone derivatives via transition-metal catalysis has been developed. Although the new methods with phthalazinone derivatives via transition-metal catalysis developed, they have been used on the C−C bond formation with π-unsaturate substrates and *N*-aryl phthalazinones limitedly. By using a transition-metal catalysis; rhodium(III) and an amide source; dioxazolones, we propose the new method the C−N bond formation of *N*-aryl phthalazinones in the catalytic C−H amination. The new method can be used in various way, especially the bioactive compound in drug discovery.



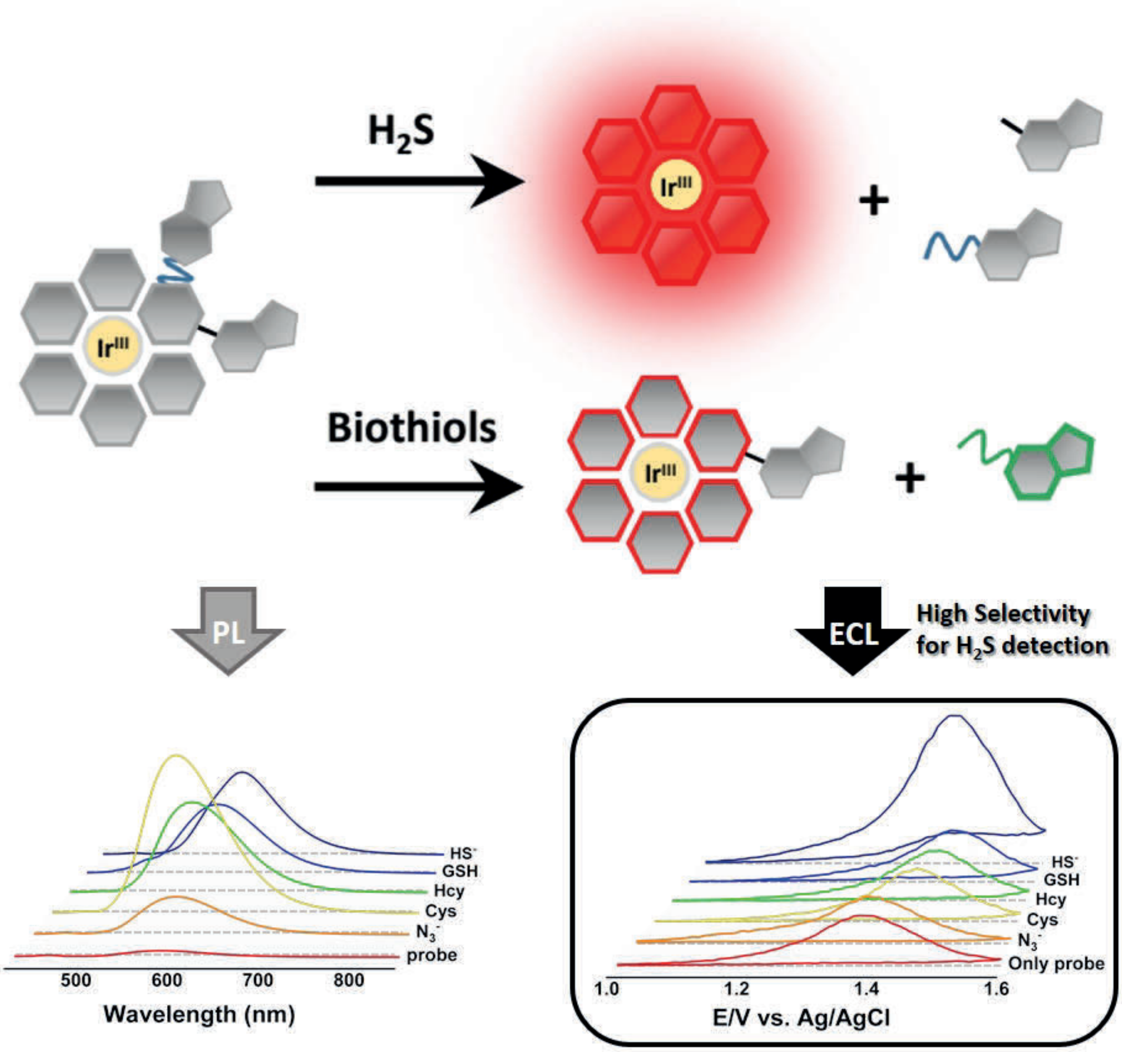
Poster Presentation : **ORGN.P-317**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Highly Selective Electrogenerated Chemiluminescence Chemodosimeter for Sulfide Enabled by Hierarchical Reactivity

Kyoung-Rok Kim, Jong-in Hong*

Division of Chemistry, Seoul National University, Korea

Electrogenerated chemiluminescence (ECL) is a luminescent process through sequential electron transfers to and from chemicals on an electrode surface. The ECL assay is advantageous compared to conventional fluorescence assay due to its high sensitivity, low background signal, and good reproducibility. Furthermore, it does not require a complicated procedure, condition and large equipment for analysis. For these reasons, ECL assay is considered as a powerful technique for on-site real sample monitoring systems.Hydrogen sulfide (H_2S) is a well-known colorless, corrosive, flammable and toxic molecule with the characteristic odor of rotten eggs. It occurs primarily in the industry, agriculture, waste disposal, and construction. Following carbon monoxide, it is the second leading toxic gas related mortality in human. H_2S is readily absorbed to humans and animals by inhalation, which causes disorders of central nervous, respiratory, cardiovascular and ocular systems. Especially, inhaling more than 500 ppm H_2S can cause permanent brain damage, coma, and even death. In addition, H_2S was used for terrorism or suicide because of easy synthesis with household ingredients. For these reasons, it is necessary to develop a real-time and accurate detection method for H_2S. Herein, we report a new ECL probe 1 based on cyclometalated iridium(III) complex rationally designed for the selective detection H_2S over various analytes including biothiols using hierarchical reactivity of the reaction sites. It showed rapid reaction rate, high sensitivity and remarkable selectivity toward H_2S, suggesting a possibility for field-monitoring. Details of photophysical and electrochemical properties will be presented.



H$_2$S
Ir^{III}
+
Biothiols
Ir^{III}
+
Ir^{III}
PL
ECL
High Selectivity for H$_2$S detection
HS$^-$
GSH
Hcy
Cys
N$_3^-$
probe
500
600
700
800
Wavelength (nm)
HS$^-$
GSH
Hcy
Cys
N$_3^-$
Only probe
1.0
1.2
1.4
1.6
E/V vs. Ag/AgCl

Poster Presentation : **ORGN.P-318**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of TKX-50 via a Protected Diazidoglyoxime Intermediate

Heun-Jong Ha, Sugyeong Kim, Kuktae Kwon[1], SeungHee Kim[1], Chang-Woo Cho[*]

Department of Chemistry, Kyungpook National University, Korea
[1] *Agency for Defense Development, Korea*

Tetrazole-based energetic materials have received considerable attention and have been intensively researched as high-energy density materials for military and civilian purposes. Dihydroxylammonium 5,5'-bistetrazole-1,1'-diolate (TKX-50) has been developed by the Klapötke group as a novel explosive based on the tetrazole *N*-oxide skeleton. TKX-50 exhibits an excellent performance, a low sensitivity, and a low toxicity, thereby drawing a lot of attention as a promising alternative to 1,3,5-trinitro-1,3,5-triazinane, which is currently the most widely used military explosive. Although TKX-50 has been effectively synthesized over five steps using glyoxal as the starting material, this synthetic route proceeds via a very sensitive diazidoglyoxime intermediate with high risk of safety-related accidents. In addition, the sensitivity of diazidoglyoxime renders it difficult to scale up the synthesis of TKX-50. Therefore, the significance of a safe synthesis of TKX-50 using diverse insensitive intermediates, instead of the sensitive diazidoglyoxime intermediate, has been established. Here, we report the safe synthesis of TKX-50 using 2-methoxyisopropyl-protected diazidoglyoxime as a promising insensitive intermediate.

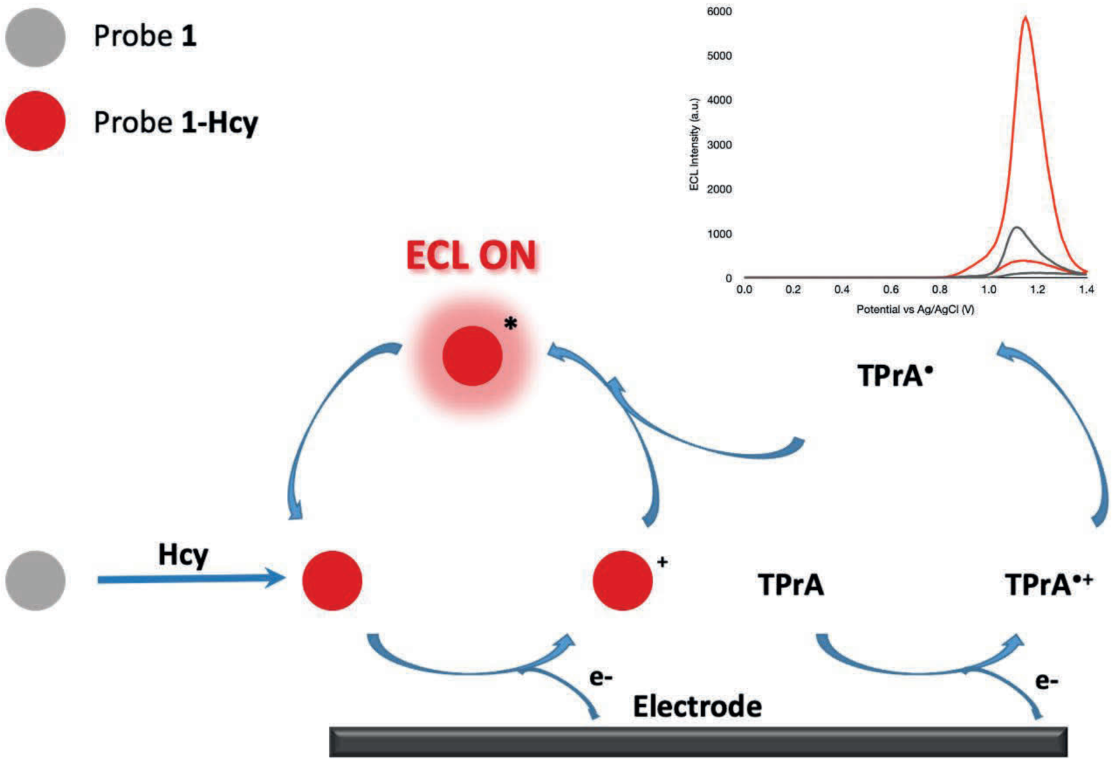
Poster Presentation : **ORGN.P-319**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

An electrochemiluminescent sensor based on cyclometalated-iridium(III) complex bearing Cu-DPA for selective turn-on detection of homocysteine

Ching-Chun Su, Jong-in Hong[1,*]

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

Homocysteine (Hcy) is an essential thiol-containing amino acid which plays a critical role in human body. It is biosynthesized from methionine via folate and vitamin B12 dependent metabolic pathways. Multiple research has suggested that total homocysteine level (tHcy) can serve as a predictive factor for various diseases. While typical concentration of homocysteine in human plasma falls between 5 to 15 uM, abnormal level of Hcy is closely related to Alzheimer's disease, renal disease, cardiovascular diseases, and neural tube defects. However, discriminating Hcy from other similarly structured biothiols such as cysteine (Cys) or glutathione (GSH) remains a difficult task.Thus, accurate and selective detection of Hcy level in biological systems is of great importance.Electrochemiluminescence (ECL) is a process where electrochemicallly generated radicals ions at the electrode surface produce light by undergoing electron transfer processes. The method is well-known for its exceptional sensitibility, accessibility and not requiring bulky optical equipments, hence its superiority over traditional fluorescence techniques. Taking advantage of these features, ECL became a well-qualified method for point-of-care testing (POCT), a prompt and precise sensing of biomarkers or chemicals. We herein report a phenylphanthridine (pphent) cyclometalated-Ir(III) complex based turn-on ECL sensor for selective Hcy detection. The complex contains a copper(II)-chelating dipicolylamine (DPA) moiety which contributes to the originally quenched luminescence. The red luminiscence was subsequently retrieved upon addition of homocysteine, while other biothiols and amino acids led to negligible response. Details of synthesis, photophysical and electrochemical properties will be presented.


Probe 1
Probe 1-Hcy
ECL ON
*
6000
5000
4000
3000
2000
1000
0
ECL Intensity (a.u.)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
Potential vs Ag/AgCl (V)
TPrA$^{\bullet}$
Hcy
+
TPrA
TPrA$^{\bullet+}$
e-
Electrode
e-

Poster Presentation : **ORGN.P-320**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

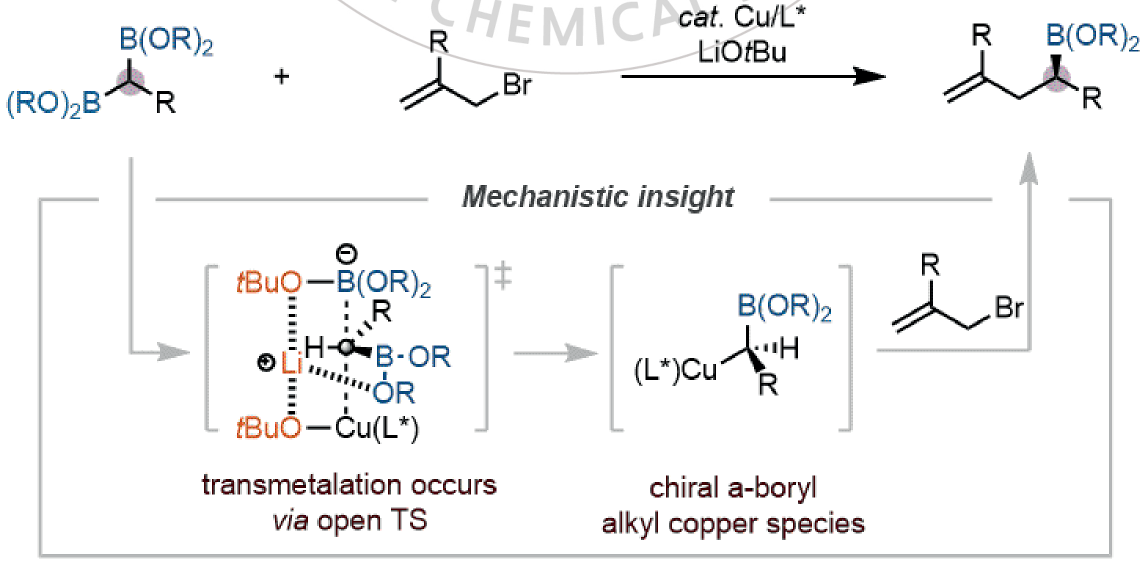
Copper-Catalyzed Enantiotopic-Group-Selective Allylation of *gem*-Diborylalkanes

Seung Hwan Cho*, **MinJae Kim**[1]

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

[1]*chemistry, Postech, Korea*

We report a copper-catalyzed enatiotopic-group-selective allylation of *gem*-diborylalkanes with allyl bromides. The combination of copper(I) bromide and H_8-BINOL derived phosphoramidite ligand proved to be the most effective catalytic system to provide various enantioenriched homoallylic boronate esters, containing a boron-substituted stereogenic center that is solely derived from *gem*-diborylalkanes, in good yields with high enantiomeric ratios under mild conditions. Experimental and theoretical studies have been conducted to elucidate the reaction mechanism, revealing how the enatiotopic-group-selective transmetalation of *gem*-diborylalkanes with chiral copper complex occurs to generate chiral α-borylalkyl copper species for the first time. Additional synthetic applications to the synthesis of various chiral building blocks are also included



Poster Presentation : **ORGN.P-321**

Organic Chemistry

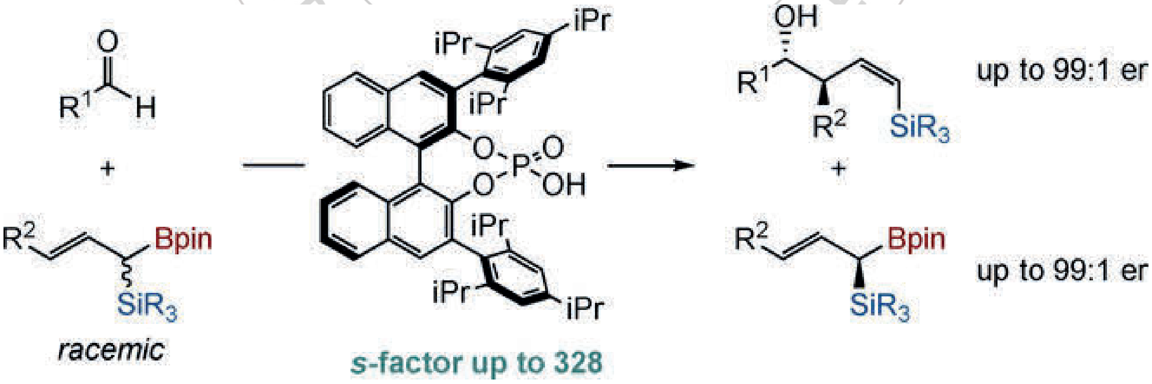
Exhibition Hall 1 FRI 11:00~12:30

Kinetic Resolution of α-Silyl-Substituted Allylboronate Esters via Chemo- and Stereoselective Allylboration of Aldehydes

Yongsuk Jung, Seung Hwan Cho*

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

We describe the kinetic resolution of α-silyl-substituted allylboronate esters via chiral phosphoric acid-catalyzed chemo-, diastereo- and enantioselective allylboration of aldehydes. This process provides two synthetically versatile enantioenriched compounds, (Z)-δ-silyl-substituted anti-homoallylic alcohols and α-silyl-substituted allylboronate esters, with a selectivity factor up to 328. We propose that the reaction proceeds through a closed chair-like transition state with the silane moiety occupying a pseudo-axial position, thus readily resolving α-silyl-substituted allylboronate esters. The synthetic utility of the obtained enantioenriched compounds is highlighted by their further transformations to give a diverse set of enantioenriched molecules.



Poster Presentation : **ORGN.P-322**

Organic Chemistry

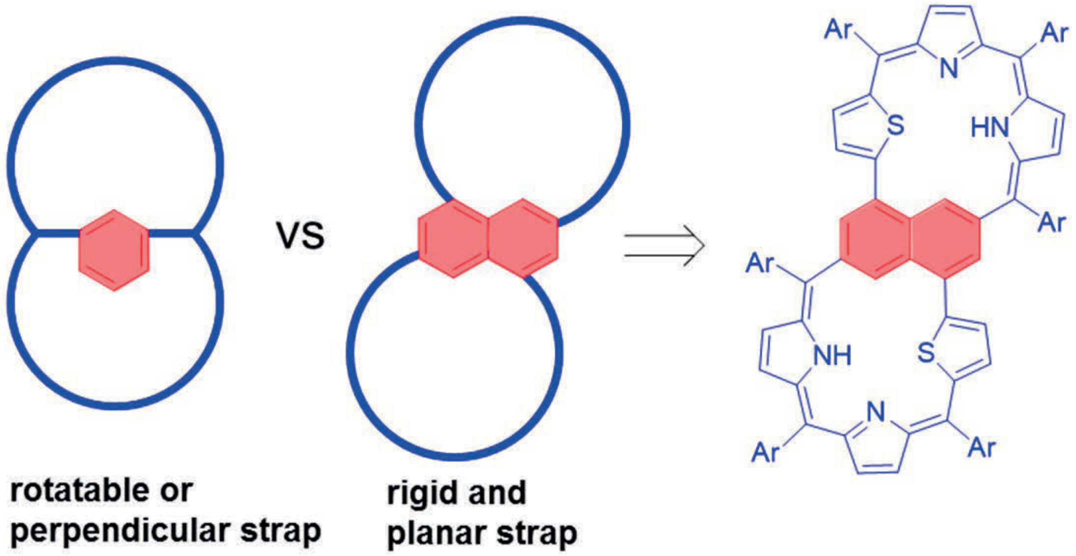
Exhibition Hall 1 FRI 11:00~12:30

Carbaporphyrin Dimers that Bear a Rigid Naphthalene Motif as an Internal Strap

Jung-Ho Hong, Dong-gyu Cho*

Department of Chemistry, Inha University, Korea

The first fully connected aromatic carbaporphyrin dimer (6) and its bis-Pd complex (6-Pd2) that bear a rigid naphthalene motif as an internal strap were synthesized. These dimers consisted of two aromatic carbaporphyrins that shared a naphthalene motif. The π-electron conjugation of the obtained macrocycles was proposed to have two separated local 22 π-electron pathways and a 34 π-electron pathway. Their weak aromaticity was fully supported by 1H NMR spectroscopy, NICS values, ACID calculations and ICSS plots.



Poster Presentation : **ORGN.P-323**

Organic Chemistry

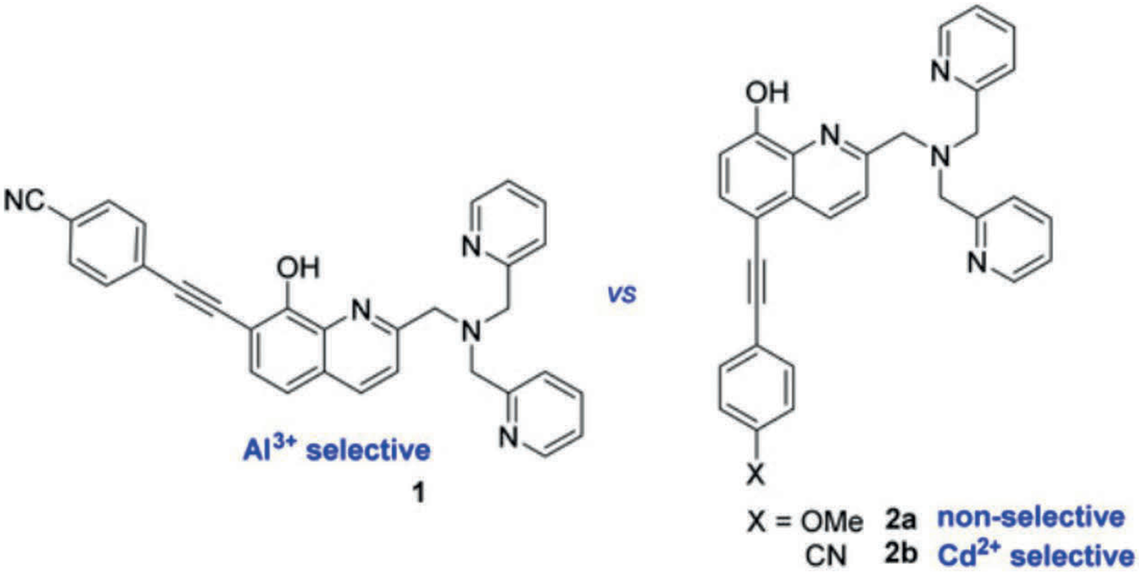
Exhibition Hall 1 FRI 11:00~12:30

Tuned Cd2+ Selectivity: Showcase of Electronic and Regio-Effect of π-Extended Di-2-Picolylamine-Substituted Quinoline-Based Tolans

Min-Sung Ko, Dong-gyu Cho*

Department of Chemistry, Inha University, Korea

π-Extended di-2-picolylamine (DPA)-substituted 8-hydroxyquinoline (8-HQ) tolans (2) were syn-thesized for testing electronic and regio-effects. The electron-poor CN-tolan (2b) showed clear se-lectivity for Cd2+ (>>Zn2+) over other metal ions via turn-on fluorescence, while the electron-rich MeO-tolan (2a) displayed no clear metal selectivity. Furthermore, considering that there was no significant energy difference between the Cd2+ complexes of 1 and 2b, the intended regio-effect (7- vs. 5-substituted effect) did not induce steric hindrance. Thus, the regio-effect is mainly electronic. Considering the above, 2a and 2b constitute a complete showcase in which electronic and re-gio-effects modulate the metal selectivity. The fluorescence titration of 2b (10 μM) with Cd2+ showed that the limit of detection (LOD) of the Cd2+-selective 2b was 158 nM in PBS (phosphate-buffered saline) (10 mM, pH 7.2) containing 50% MeOH.



Poster Presentation : **ORGN.P-324**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Highly Selective, Sensitive and Reusable Colormetric Chemosensor for Naked-eye Detection of Hydrogen Sulfide under Versatile Conditions

Na Young Cho, Byeong M. Oh, Jong Hyun Kim*

Department of Molecular Science and Technology, Ajou University, Korea

In this presentation, we report a new colorimetic chemosensor based on Benzodipyrrolidone moiety for the detection of hydrogen sulfide (H2S). which can affect injurious defect to human body. Highly sensitive (limit of detection : 1.56uM) and selective reactivity of BDP-Br enables colorimetric response of the BDP-Br solution to the H2S by showing well-defined visible color change from yellow to colorless. We also have investigated BDP-Br does not show any differences with analytes including thiol group in UV-vis absorption so that it can be worked as high selective H2S chemosensor. Based on systemic characterizations, including UV-vis absorption and NMR spectral analyses, we revealed that BDP-Br return to precursor when it reacts with H2S. This advantageous property suggests that BDP-Br can be practically applicated for reusable chemosensor under versatile conditions.

Poster Presentation : **ORGN.P-325**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

CuPC-based Synergist for Blue Color Photoresist

Eun Hye Lee, Byeong M. Oh, Na Young Cho, Jong Hyun Kim*

Department of Molecular Science and Technology, Ajou University, Korea

In this presentation, we report CuPC-based synergist molecules for blue color photoresist. Correlationship among substituted terminal functional units, optical properties, and thermal properties will be presented.

Poster Presentation : **ORGN.P-326**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Room Temperature *N*-Formylation of Secondary Amines using Methanol as a C_1 Source Catalyzed by Reusable Bimetallic AuPd–Fe_3O_4 Nanoparticles

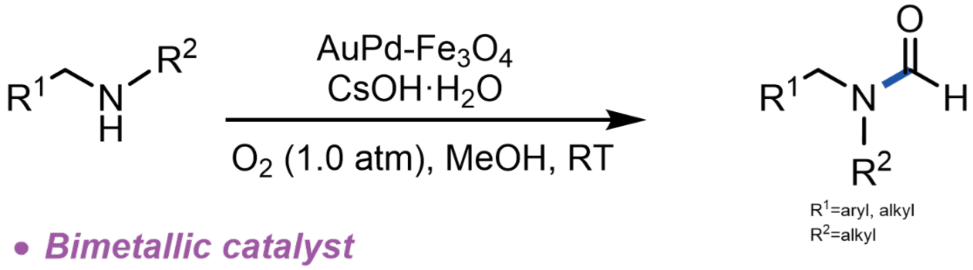
Sabyuk Yang, Byeong Moon Kim[*]

Department of Chemistry, Seoul National University, Korea

Development of facile formamide synthesis has been extensively studied because of its prevalence in organic and pharmaceutical chemistry. Among various pathways to formamide, attaching a formyl group directly to an amine is one of the most straightforward routes. However, many synthetic protocols developed so far generally require toxic reagents such as cyanide, formic acid, formate ester, and so on. To circumvent the use of these harmful reagents, chemists have focused on methanol as an ideal C_1 source due to its availability, sustainability, low toxicity, and low cost. A handful of catalytic methods have been developed for the *N*-formylation process, including homogeneous and heterogeneous catalysts containing transition metals.

Heterogeneous catalysts have been regarded as an alternative to homogeneous catalysts due to its recyclability and stability. In this research, we report a new synthetic procedure of formamide synthesis using a recyclable AuPd–Fe_3O_4 bimetallic catalyst. The reactions were carried out under atmospheric pressure of O_2 at room temperature, which is by far the mildest condition compared to other similar works. The nanocatalyst can be recovered and reused for more than 10 times without a significant loss of its activity.

References
[1] A. Cho, S. Byun, B. M. Kim, *Adv. Synth. Catal* **2018**, *360*, 1253–1261.
[2] A. Cho, S. Byun, J. H. Cho, B. M. Kim, *ChemSusChem* **2019**, *12*, 2310–2317.



- ***Bimetallic catalyst***
- ***Catalyst recyclable for 12 times***
- ***Mild condition (1.0 atm of O_2, room temperature)***
- ***High yield & broad substrate scope***

Poster Presentation : **ORGN.P-327**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

pH-sensitive Organic Dye and its Application as Security Ink for Information Encryption on Paper

Won-Sik Han[*], Yeeun Lee

Department of Chemistry, Seoul Women's University, Korea

Tunable solid-state fluorescent materials based on donor–acceptor systems have great potential for sensing applications. In this work, two donor–acceptor type molecules, 3,6-di(*9H*-carbazol-9-yl)pyridazine **(CzPyr–H)** and 3,6-bis(3,6-dimethoxy-*9H*-carbazol-9-yl)pyridazine **(CzPyr–OMe)**, were designed and synthesized to study their volatile acid detection ability. The photophysical properties of **CzPyr–H** and **CzPyr–OMe** were systematically investigated along with density functional theory calculations. As protonating central pyridazine unit, an absorption band at the longer wavelength was broadened owing to intramolecular charge transfer (ICT). Furthermore, the emission intensity gradually decreased with increasing TFA concentration, which indicate that these compounds can be used in acid sensing application. In their aggregated states, both compounds showed aggregation-enhanced emission (AEE) characteristics. Finally, **CzPyr–H** and **CzPyr–OMe** were successfully applied as fluorescent probes for volatile acid detection and as security ink for information encryption on paper, utilizing their TFA sensitivity and the AEE character.

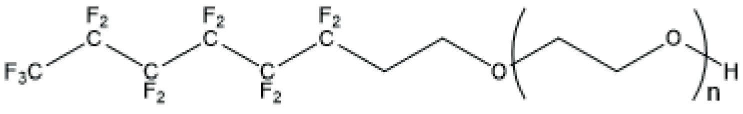
Poster Presentation : **ORGN.P-328**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Adducts of perfluorohexyl ethanol with ethylene oxide were characterized by spectroscopic methods and the interfacial tensions of the adducts were measured in terms of the number of EO units.

Myoung-Hoon Kim, Eun Sil Kim[1], Surk-Sik Moon[2,*], Byeong Jo Kim[3], Hyun-chul Kang[4], Chan Kyu Kwak[4], Won-Jun Jeong[4]

Department of chemistry, Kongju National University, Korea
[1]*Kongju National University, Korea*
[2]*Department of Chemistry, Kongju National University, Korea*
[3]*R&D Center, AK CHEMTECH, Korea*
[4]*Surfactant R&D team, AKCHEMTECH, Korea*

The reaction mixture of perfluorohexyl ethanol with ethylene oxide was fractionated by silica gel chromatography (Silica MPLC) to provide each perfluorohexyl alcohol-ethylene oxide adduct. Each component was characterized by using spectroscopic methods including 1D and 2D NMR (COSY, HSQC and HMBC) spectroscopy. The average number of ethylene oxide (EO) unit in the fractions was estimated by NMR analysis. Interfacial tensions of each fractions were measured to provide the optimum number (EO = 5 ~ 6) of EO units in the adducts.



Perfluorohexyl ethanol-(EO)n

Poster Presentation : **ORGN.P-329**

Organic Chemistry

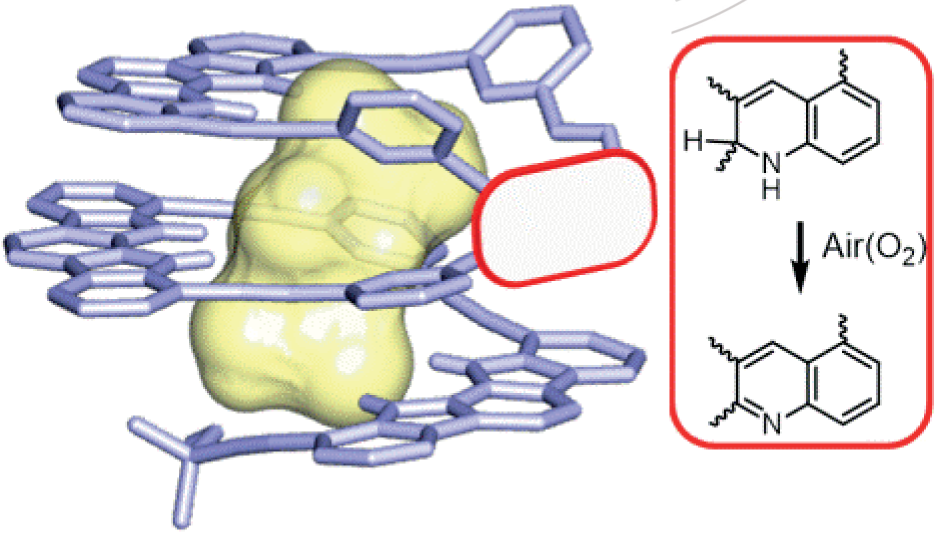
Exhibition Hall 1 FRI 11:00~12:30

Effects of Subtle Receptor Modifications on the Affinities and Selectivities for Binding Chiral Guests

Geunmoo Song, Kyu-Sung Jeong*

Department of Chemistry, Yonsei University, Korea

Recently, we reported optically pure aromatic foldamers via template directed one-pot synthesis. These aromatic foldamers were fixed in helix orientation by covalent locking of helical backbones, and showed selective binding for chiral templates (D- or L-tartaric acid, or D- or L-sorbitol).[1] These helical receptors contained labile 1,2-dihydroquinoline ring in the backbone, which in this study were oxidized to the thermodynamically stable quinoline ring. Despite similar folding structures and cavities before and after subtle modifications, these helical receptors exhibited surprisingly different affinities and selectivites for binding chiral guests.[2] All details including synthesis, single crystal X-ray structures, ^{1}H NMR studies, CD titrations, and thermodynamic parameters will be described in the presentation.References[1] K. M. Kim,† G. Song,† S. Lee, H.-G. Jeon, W. J. Chae, K.-S. Jeong, Angew. Chem. Int. Ed. 2020, 59, 22475-22479. († co-first authors)[2] G. Song, K. M. Kim, S. Lee, K.-S. Jeong, Chem. Asian J. Doi.org/10.1002/asia.202100768.



Poster Presentation : **ORGN.P-330**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Liquid Phase Synthesis of Peptide Nucleic Acid Trimers and their Assembly on MBHA resin of Purine Rich gamma PNA Oligomer Sequence

Alagarsamy Periyalagan, In seok Hong[1,*]

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

Emerging applications of Peptide Nucleic Acid (PNA) oligomers encouraged probe of rapid and efficient synthesis of PNA oligomers. Solid Phase peptide synthesis (SPPS) is the most convenient method of synthesizing PNA Oligomers by sequential coupling of the corresponding monomers. However, the final synthesis yield is limited when synthesizing an extended or oligomer with specific continuous base sequences. Here we report an efficient protocol for PNA oligomers synthesis using fully protected PNA trimers instead of monomers. Consequently, it reduces the number of coupling cycles during SPPS by about 66% and increased relatively high HPLC purity. Here the trimers were prepared by using Liquid Phase Peptide Synthesis (LPPS). In this reported protocol, the gamma lysine PNA Oligomer with 13 base lengths, including 77% purine content, has been examined.

Poster Presentation : **ORGN.P-331**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

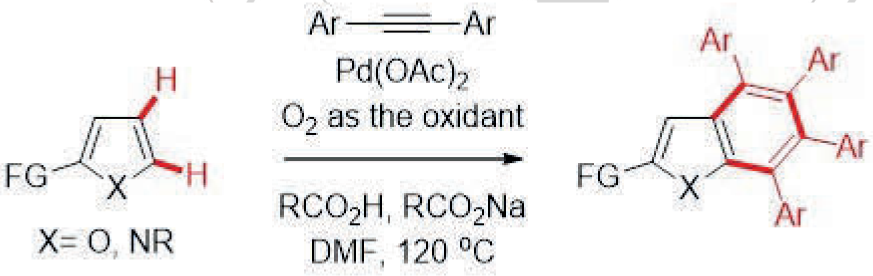
Pd-Catalyzed Aerobic Benzannulation of Furans and Pyrroles with Alkynes

Jia Seo, Jung Min Joo[1,*]

chemistry, Pusan National University, Korea

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

Furans and pyrroles stabilized by electron-withdrawing groups underwent Pd-catalyzed 1:2 annulation reaction with diaryl alkynes. The presence of synthetically useful electron-withdrawing groups stabilized the electron-rich heterocycles and promoted C–H functionalization reactions. It was successfully annulated by the Pd catalytic system. Moreover, the combination of 2,2-dimethylbutyric acid and its conjugate base facilitated metalation at the heteroaromatic rings and reoxidation of the Pd(0) species using oxygen as the terminal oxidant.



Poster Presentation : **ORGN.P-332**

Organic Chemistry

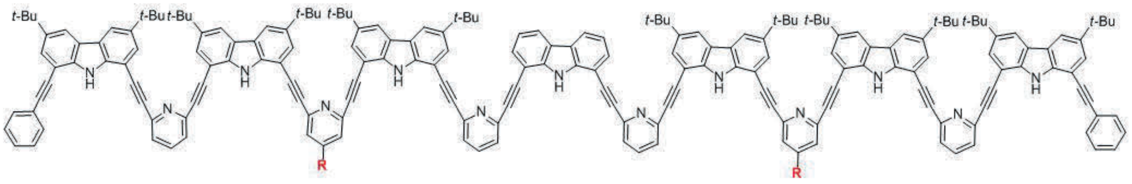
Exhibition Hall 1 FRI 11:00~12:30

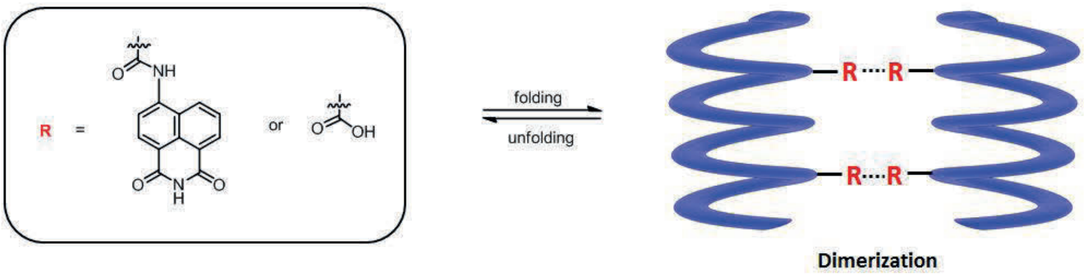
Helix-to-Helix Interactions between Carbazole-Pyridine Hybrid Foldamers

Hye Jin Jang, Kyu-Sung Jeong[*]

Department of Chemistry, Yonsei University, Korea

We prepared carbazole-pyridine (CP) hybrid oligomers that can adopt helically folded conformations in solution and in the solid states. The helical folding of these CP oligomers was driven primarily by local dipole-dipole interactions between the two repeating monomers linked through the ethynyl bond. At the outside periphery of the CP helices, functional groups such as carboxylic acid and imide were introduced to promote helix-to-helix interactions, thus affording helix dimers. These CP foldamers were investigated to function as synthetic receptors to bind complementary guests in their binding sites. Details including syntheses, structural analyses and binding studies will be discussed in the poster presentation.





Poster Presentation : **ORGN.P-333**

Organic Chemistry

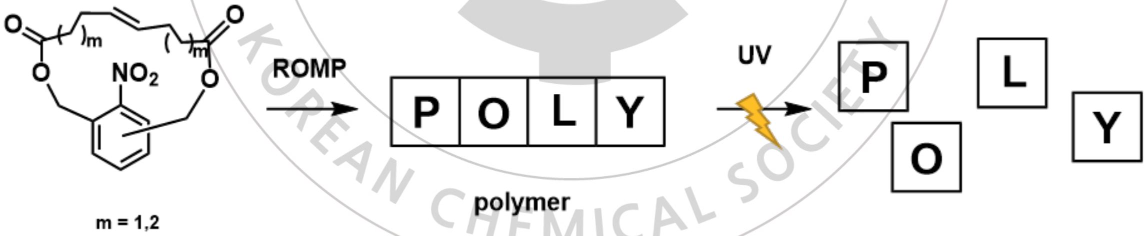
Exhibition Hall 1 FRI 11:00~12:30

Study for Synthesis and Degradation of Photo-Cleavable Polymers via ROMP from Structurally Different *ortho*-Nitrobenzyl Esters

Bon Woo Koo, Dopil Kim, Min Kim*, Cheoljae Kim*

Department of Chemistry, Chungbuk National University, Korea

The photocleavable polymers have been developed via ring-opening metathesis polymerization (ROMP) using Grubbs catalyst. The newly designed monomers have an ortho-nitrobenzyl ester functional group, and six different isomers, *i.e.* *ortho*-, *meta*- and *para*-monomers with different ring sizes, were demonstrated for the polymerization with Grubbs catalysts and degradation under UV light. 17-membered meta-monomer was the most reactive, and various polymers were synthesized. We are continuously studied for the application of this photocleavable polymers for changing their physical properties.



Poster Presentation : **ORGN.P-334**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Renewable Catalytic Reaction: Conversion of Carbohydrates to 2,5-Diformylfuran

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

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

Biomass is highlighted as the most promising alternative to depleting fossil resources. Lignocellulosic biomass, the abundant carbon pool, is anticipated to play a crucial role in the supply of various chemicals and fuels through catalysis. Naturally occurred C5 and C6 sugars can be converted to furan molecules such as 5-hydroxymethylfuran (HMF). 2,5-Diformylfuran (DFF) is produced from the oxidation of HMF, has potential applications as a monomer of polymers, heterocyclic ligands, luminophores, and platform chemicals. Recently, there have been plentiful reports for the synthesis of DFF from fructose. However, these methods are under high temperature (150 °C) or involving several steps: dehydration of fructose to HMF with Brønsted acid, and generation of DFF through the oxidation of HMF. In this study, we report one-step approach transforming various carbohydrates such as fructose, glucose, sucrose to DFF with high yields under mild conditions.

Poster Presentation : **ORGN.P-335**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and photophysical properties of thiophen-modified methyl salicylate derivatives

Nam wook Kim, Intae Kim[1,*], Jun-Gill Kang[2,*]

Department of Chemistry, KWANG WOON university, Korea
[1]*Department of Chemistry, Kwangwoon University, Korea*
[2]*Department of Chemistry, Chungnam National University, Korea*

We have studied newly synthesized methyl salicylate derivatives with hetero aromatic compounds. Methyl salicylate and its derivatives are naturally found in plants and foods, and used as ingredients of medicinal products, food, mouthwash, and surrogate of chemical warfare agents. Because methyls salicylate has similar properties with other chemical warfare agents like soman and sulfur mustard, methyl salicylate and its derivatives have important role for surrogate of chemical warfare agents.Previously, we found that the substitution of methoxy or cyno at 5 position of the thiophenyl moiety in methyl 2-hydroxy-4-(thiophen-2-yl)benzoate (MHTB) results in very unique luminescence properties, such as highly enhanced quantum yield (Φ) and solvatochromism, depending on the substituted group. The electron-donating methoxy group markedly enhances the quantum yield (Φ = 86.7%), compared with the electron-withdrawing cyano group (Φ = 9.2%). In this study, methyl 2-hydroxy-4-(5-methoxythiophen-2-yl)benzoic acid (MHmoTBA) has been synthesized and its photophysical properties are examined in dichloromethane, dimethyl sulfoxide (DMSO) and methanol (MeOH).Based on the above contents, the physical properties of the various methyl salicylate derivatives were found through this study, and the comparative properties of methyl salicylate and its new derivatives were also studied.key words : methyl salicylate, hetero aromatic compounds, methyl salicylate derivatives

Poster Presentation : **ORGN.P-336**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A study on the characteristics of peptide coupling reaction using Bts-based gamma PNA monomers

Jiseon Kim, Seonjin Kim[1], In seok Hong[2,*]

Chemistry, Kongju National University, Korea
[1]*Kongju National University, Korea*
[2]*Department of Chemistry, Kongju National University, Korea*

Peptide nucleic acid (PNA) oligomers have traditionally been synthesized in the solid phase using either the Fmoc or Boc protecting group strategy. In 2007, a Bts protecting group-based synthesis method was reported in the literature, and in that method, the transacylation was inhibited, so that PNA oligomers could be synthesized in high yield and purity. In addition, when gamma-modified PNA was introduced into a PNA oligomer, there have been many reports of increased binding strength and selectivity to DNA. However, a method for synthesizing a gamma PNA monomer based on a Bts protecting group has not yet been reported. In this study, Bts-based gamma PNA monomers with side branches such as alanine, glutamic acid, and lysine were synthesized and peptide reaction characteristics were studied in the dimer model.

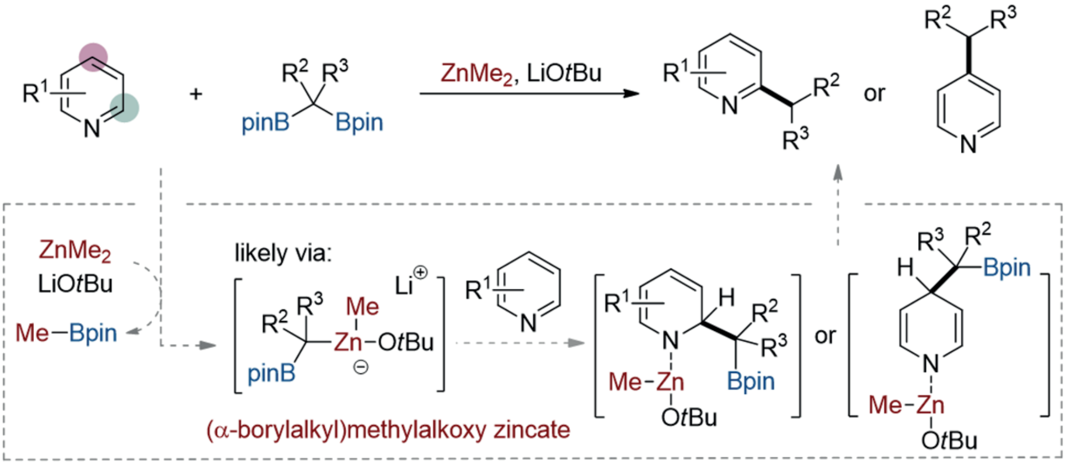
Poster Presentation : **ORGN.P-337**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

ZnMe2-Mediated, Direct Alkylation of Electron-Deficient N-Heteroarenes with 1,1-Diborylalkanes: Scope and Mechanism

Woohyun Jo, Seung Hwan Cho*

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

The regioselective, direct alkylation of electron-deficient N-heteroarenes is, in principle, a powerful and efficient way of accessing alkylated N-heteroarenes that are important core structures of many biologically active compounds and pharmaceutical agents. Herein, we report a ZnMe2-promoted, direct C2- or C4-selective primary and secondary alkylation of pyridines and quinolines using 1,1-diborylalkanes as alkylation sources. While substituted pyridines and quinolines exclusively afford C2-alkylated products, simple pyridine delivers C4-alkylated pyridine with excellent regioselectivity. The reaction scope is remarkably broad, and a range of C2- or C4-alkylated electron-deficient N-heteroarenes are obtained in good yields. Experimental and computational mechanistic studies imply that ZnMe2 serves not only as an activator of 1,1-diborylalkanes to generate (α-borylalkyl)methylalkoxy zincate, which acts as a Lewis acid to bind to the nitrogen atom of the heterocycles and controls the regioselectivity, but also as an oxidant for rearomatizing the dihydro-N-heteroarene intermediates to release the product.



Poster Presentation : **ORGN.P-338**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

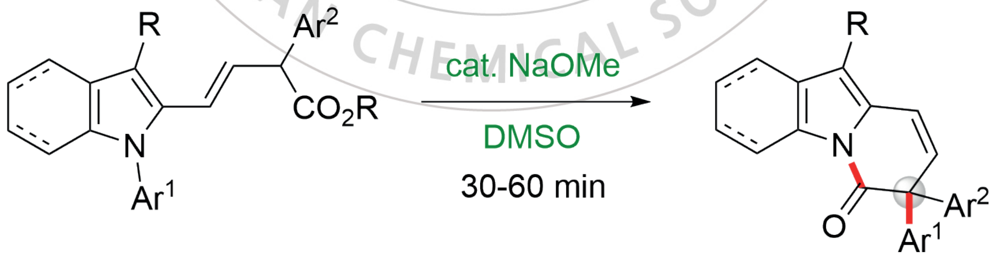
Methoxide as Metal-free Catalyst for the Synthesis of Pyrido[1,2-*a*]indolones

Sun-a Park, Juhyun Kim*

Department of Chemistry, Gyeongsang National University, BK 21 FOUR, Research Institute of Natural Science, Korea

A simple metal-free strategy for the synthesis of pyrido[1,2-*a*]indolone derivatives has been devised through sodium methoxide-catalyzed intramolecular cyclization of 2-alkenylated *N*-pyrimidyl indoles. The reactions involved a Smiles rearrangement/cyclization cascade, which resulted in a new series of *N*-fused indoles, potentially applicable skeletons in medicinal chemistry. This reaction presents simple eco-friendly reaction conditions, a high atom- and cost-economy, a short reaction time, and a broad range of scope with high reaction efficiency.

This work: Metal-free method for the synthesis of DHPI derivatives



- *Metal-free*
- *Short reaction time*
- *Re-use of leaving group as a catalyst*
- *Simple reaction conditions*
- *Without extra additives*
- *Gram-scale synthesis*

Poster Presentation : **ORGN.P-339**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

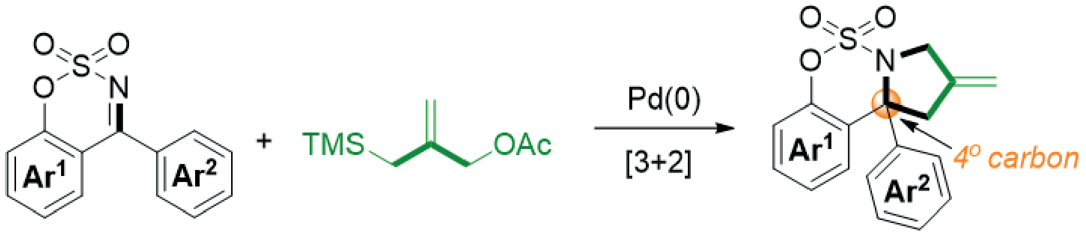
Access to Fused Pyrrolidines bearing a Quaternary Carbon via Pd-Catalyzed [3+2] Cycloaddition of Sulfamate-derived Ketimines with Trimethylenemethanes

Seoung-Mi Choi, Juhyun Kim*

Department of Chemistry, Gyeongsang National University, BK21 FOUR, Research Institute of Natural Science , Korea

The quaternary carbon centered pyrrolidine is ubiquitous in the architectures of numerous natural products, bioactive molecules and pharmaceuticals. On the other hand, the sulfamate moiety has also specific biological activities, such as anticancer, antibiotic, and antiviral acitivity, and serves as reactive intermediate that can be readily converted to other useful heterocycle. Therefore, developing new method for the synthesis of compounds incorporating both sulfamate and quaternary carbon centered pyrrolidine moieties is highly significant. In this work, we have developed Pd-catalyzed [3+2] cycloaddition to access sulfamate-fuctionalized pyrrolidines bearing a quaternary carbon center, starting from readily available trimethylenemethane (TMM) and sulfamate-derived cyclic ketimines.

This work



1 Cyclic Ketimine

2 TMM

3

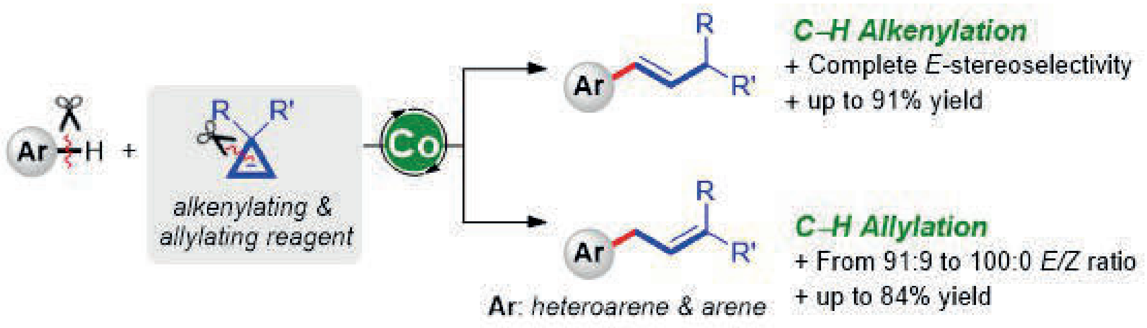
Poster Presentation : **ORGN.P-340**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Co^{III}-Catalyzed C–H Alkenylation and Allylation with Cyclopropenes via Sequential C–H/C–C Bond Activation

Yelim Kim, Juhyun Kim[1,*]

Department of Chemistry, Gyeongsang National University, BK 21 FOUR, Research Institute of Natural Science, Korea
[1]*Department of Chemistry , Gyeongsang National University, BK 21 FOUR, Research Institute of Natural Science, Korea*

Atom-economical strategies that can synthesize useful compounds while minimizing the byproducts are among the most important goals of sustainable chemistry. In this regard, catalytic methodologies that functionalize ubiquitous C–H or C–C bonds in hydrocarbons have gained considerable momentum over the past decades. To maximize the atom-economy and overcome the difficulty of activating inert catalytic C–C bonds, sequential C–H/C–C bond activation strategy has recently attracted attention. After a few years of efforts with a precious Rh catalyst, the paradigm has shifted toward the development of environmentally benign first-row transition metal catalyzed transformations involving C–H/C–C bond activation. Herein, we have developed a highly efficient and atom-economical protocol for the cobalt-catalyzed C–H alkenylation of (hetero)arenes, enabling cyclopropenes as alkenylating reagents. This cobalt catalysis, involving C–H bond activation/olefin insertion into a cyclopropene/C–C bond cleavage sequence, features a broad spectrum of substrates including heteroarenes and simple arenes, good functional group tolerance, high efficiency, and complete *E*-stereoselectivity. The same catalytic system was successfully applied for double isomerization of the initially formed alkenyl (hetero)arenes. By adding excess base, allylated (hetero)arenes with excellent *E*-stereoselectivity were obtained (*E*/*Z* ratio = 91:9 to 100:0). This cobalt catalysis is characterized by the uses cyclopropenes as new alkenylating and allylating reagents in C–H activation using C–H/C–C bond activation strategy.


Ar
H
R
R'
alkenylating & allylating reagent
Co
Ar
R
R'
C–H Alkenylation
+ Complete E-stereoselectivity
+ up to 91% yield
Ar
R
R'
Ar: heteroarene & arene
C–H Allylation
+ From 91:9 to 100:0 E/Z ratio
+ up to 84% yield

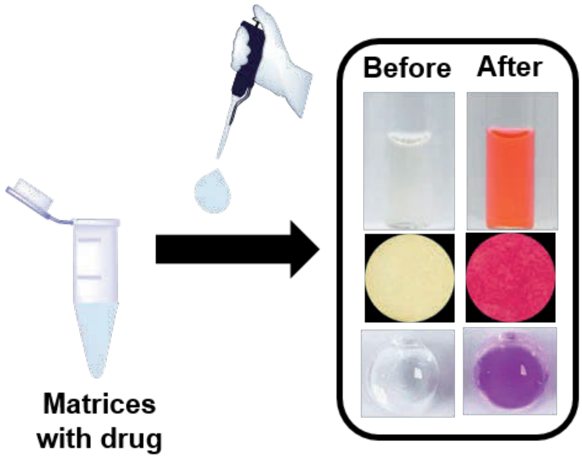
Poster Presentation : **ORGN.P-341**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Simple and fast colorimetric detection for amphetamine type illicit drugs

<u>Siyoung Cho</u>, Youngmi Kim[1,*]

chemistry, Kyung Hee University, Korea
[1]*Department of Chemistry, Kyung Hee University, Korea*

Abuse of illicit drugs causes serious health and social problems. Therefore, the development of efficient analytical detection methods is urgently needed. In this presentation, a simple, fast, and low-cost method for the detection of amphetamine-type illicit drugs will be presented. Colorimetric indicator **1** was synthesized in low-cost, and it can be easily synthesized in large quantities. Compound **1** reacts predominantly with secondary amines, for example, methamphetamine, 3,4-methylenedioxymethamphetamine, and methcathinone, which induced a red shifted absorption band resulting in a color change from colorless to red-pink. This method doesn't have any interference from other pharmaceuticals, ingredients in alcoholic and non-alcoholic beverages, or additives found in street illicit drugs. **1**-based colorimetric assay was successfully applied for the detection of amphetamine-type illicit drugs in various matrices such as aqueous solutions, artificial urine samples, alcoholic/non-alcoholic beverages, and artificial ecstasy tablets. Based on the rapid color changes, **1**-based solution and solid state assays can allow the highly sensitive and selective detection of amphetamine-type illicit drugs within 2 min. This work suggests that compound **1** can be a useful colorimetric indicator for the detection of illicit drug in the field.



- ✓ Easy
- ✓ Fast
- ✓ Low cost
- ✓ Naked eye detection

Poster Presentation : **ORGN.P-342**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Organocatalytic Asymmetric Michael Addition in Aqueous Media by a Hydrogen-Bonding Catalyst and Application for Inhibitors of GABAB Receptor: Computational DFT study for mechanism and structure.

Jae Ho Shim*, Byung Kook Ahn[1], Deok-Chan Ha[2]

Department of Anatomy, Korea University, Korea
[1]*Health and Enviromental Science, Korea University, Korea*
[2]*Department of Chemistry, Korea University, Korea*

The role of an aqueous medium for organic catalytic activity can be reversed concerning hydrophilic-hydrophobic function depending on the reaction conditions. In this study, to provide an environmentally friendly system, the thiourea-based catalyst substituted with 3,5-(CF3)2-Ph was used in water solvents. The hydrophobic effect of the substituent provides fast reaction, high chemical yield, and mirror-image selectivity. This reaction allowed the preparation of GABAB agonists in an optically pure manner. Besides, GABA (γ-aminobutyric acid) analogs such as baclofen and phenibut were synthesized as R-type S-type with high optical purity.

Poster Presentation : **ORGN.P-343**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

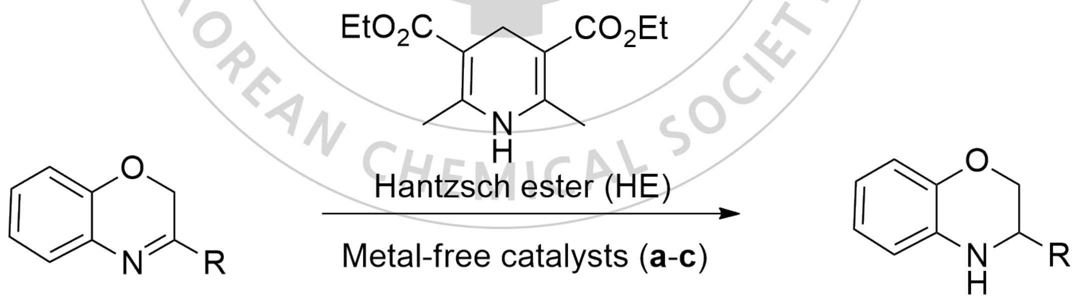
Development of the isothiouronium salt type organic catalyst for Efficient Synthesis of Various 3,4-dihydro-2H-1,4-benzoxazines

Sungmin Kang, Taek Hyeon Kim[*]

School of Chemical Engineering, Chonnam National University, Korea

This study reports on the isothiouronium salt catalyzed transfer hydrogenation of various 3-substituted-2H-1,4-benzoxazines with Hantzsch esters as a hydrogen source. Transfer hydrogenation of 3-substituted-2H-1,4-benzoxazines has been successfully realized with 1 mol% of S-benzyl-N, N'-diphenyl isothiouronium iodide as the catalyst. Various of 3,4-dihydro-2H-1,4-benzoxazines were obtained in high yield in a short reaction time under mild room temperature conditions.

Previous reports on metal-free catalysts under HE



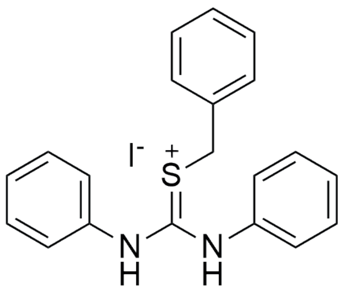
a) Phosphonic acid: *ref.5a-e*

b) $B(C_6F_5)_3$: *ref.5f*

c) Thiourea dioxide: *ref.5g*

This work

d) **Isothiouronium salt**, metal-free catalyst



Poster Presentation : **ORGN.P-344**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Cerium(III) triflate-catalyzed ring opening of epoxides : Synthesis of vesamicol and benzovesamicol

Min Ju Yun, Eunae Kim*

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

A simple and efficient method for the regioselective ring opening of epoxides with amines has been developed using a catalytic amount of cerium(III) triflate. This method was applicable to a wide range of substrates and allowed for gram-scale synthesis. In the case of cyclohexene oxide, only one isomer with trans stereochemistry was formed. The aminolysis of styrene oxide with anilines gave the major product with an attack at the benzylic position. Unfortunately, the reaction of styrene oxide with aliphatic amines gave poor regioselectivity. It was confirmed that this method is applicable to the efficient synthesis of vesamicol and benzovesamicol, known as the vesicular acetylcholine transporter (VAChT) ligands.

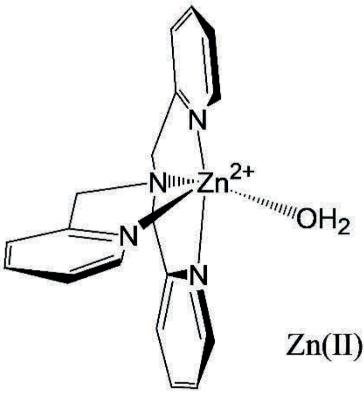
Poster Presentation : **ORGN.P-345**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mechanistic studies of the hydrolysis of carboxylic ester using Tris(2-pyridylmethyl)amine-based catalytic zinc complexes

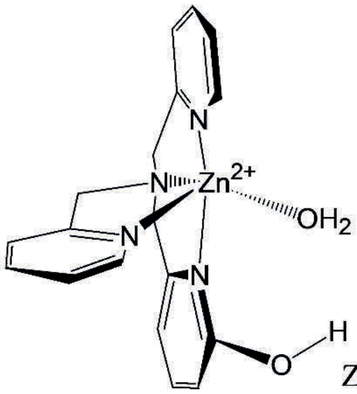
Ji Yoon Lim, Soo Suk Lee*

Department of pharmaceutical engineering, Soonchunhyang University, Korea

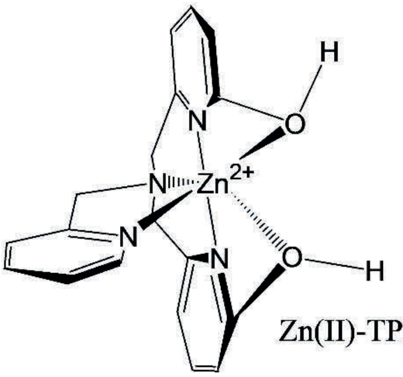
Developing efficient artificial catalysts comparable to biocatalysts such as enzymes has been a enduring challenge and difficult task that have yet to be met for researchers studying enzyme mimics for a long time. The studies reported herein is concerned with the identification of the mechanism of the ester hydrolysis reaction based on the design, synthesis and kinetic studies of zinc complexes capable of catalyzing the hydrolysis of p-nitrophenyl acetate. Tris(2-pyridylmethyl)amine (TPA) is a typical tripodal tetradentate amine ligand that is frequently used to mimic the active site environment of enzymes by the formation of TPA-metal ion complexes with various metal ions. TPA-metal ion complexes are synthesized as enzyme mimics and used as catalysts for many chemical reactions including hydrolysis of carboxyl esters. We have demonstrated that the reactivity is increased or decreased by the introduction of a hydroxymethyl group into the TPA ligand in relation to the coordination structure of the zinc complex based on the single crystal structure. According to the coordination structure of zinc complexes, we propose a novel mechanism in contrast to the previous explanation that the hydroxyl group, which is a nucleophilic group coordinated to a metal ion, has a lower pKa value, thereby increasing the rate of the hydrolysis reaction. While the hydroxyl group does not coordinate with the metal ion and stabilizes the substrate by hydrogen bonding, thereby improving the hydrolysis reaction rate, even if the hydroxyl group binds to the metal ion, it does not act as a nucleophile, so that the hydrolysis reaction does not occur. This study suggests a novel strategy for the development of more efficient metal ion-based artificial catalysts, and suggests possible modes of action for metalloenzymes.



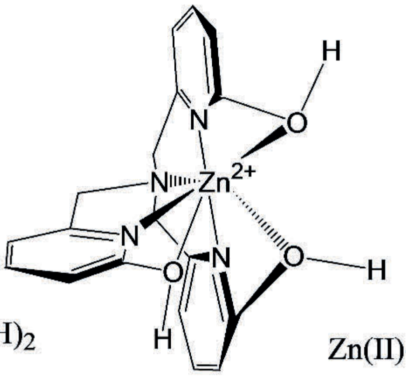
Zn(II)-TPA



Zn(II)-TPA(CH$_2$OH)



Zn(II)-TPA(CH$_2$OH)$_2$



Zn(II)-TPA(CH$_2$OH)$_3$

Poster Presentation : **ORGN.P-346**

Organic Chemistry

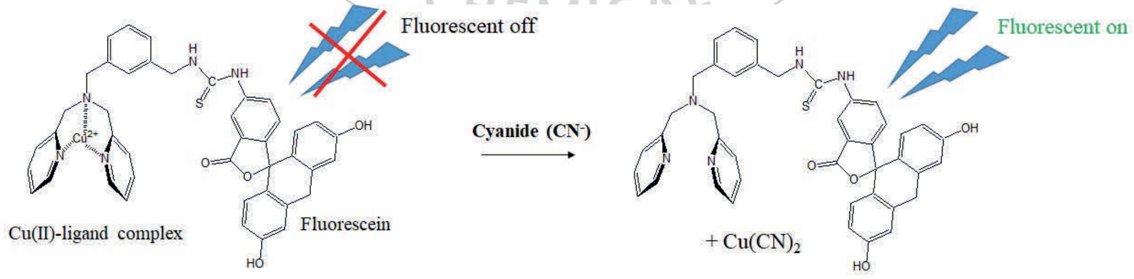
Exhibition Hall 1 FRI 11:00~12:30

Detection of cyanide ion using novel fluorescein-containing copper(II) complex

Min Ji Kim, Ji Yoon Lim, Soo Suk Lee[*]

Department of pharmaceutical engineering, Soonchunhyang University, Korea

Cyanide is an extremely toxic substance that causes fatal disease in humans. Due to severe toxicity, the World Health Organization (WHO) published a guideline value of 70 µg/L for cyanide in drinking water in 1996. Despite these fatal problems, cyanide is produced in large quantities and is commonly used in mining, industrial organic chemistry and medical applications. Therefore, over several decades, many researchers have developed cyanide detection methods. The development of a technology that can detect even a small amount of cyanide anion with specific and high sensitivity is still required, and we want to approach it with a new concept of fluorescence detection. In this study, we used a novel compound containing a ligand capable of forming a complex with a metal ion in addition to a fluorescent dye for the detection of cyanide anion. Our novel ligand and Cu(II) complex exhibited a high selectivity and sensitivity toward cyanide by changing fluorescent intensity at 514 nm.



Poster Presentation : **ORGN.P-347**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Blue Organic Light-Emitting Diodes using 11,11-dimethyl-10-(phenylanthracen-9-yl)-11H-indeno[1,2-b]quinoline derivatives

Giwoong Han, Seung Soo Yoon[1,*]

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

In organic light-emitting diodes (OLEDs), the improvement of the efficiency and lifetime of blue emitters is a problem to be solved. In this study, two blue fluorescence materials using phenylanthracene-substituted dimethyl-indenoquinoline derivatives were synthesized and characterized for OLEDs. To study their electroluminescent properties, OLED devices were fabricated in the following sequence : ITO (180 nm) / 2-TNATA (30 nm) / NPB (20 nm) / emitting materials (20 nm) / BPhen (30 nm) / Liq/Al (100 nm) using these materials as emissive layer (EML). A device using 11,11-dimethyl-4-(10-phenylanthracen-9-yl)-11H-indeno[1,2-b]quinoline in emitting layer showed the efficient blue emission with the external quantum efficiency (EQE) of 4.10 %, the luminance efficiency of 3.52 cd/A and power efficiency of 1.97 lm/W at 20 mA/cm^2. This device also showed the deep blue emission with the CIE coordinates (0.15, 0.09) at 8.0 V. This result suggests that phenylanthracene-substituted dimethyl-indenoquinoline derivatives can serve as promising blue emitters for OLEDs.

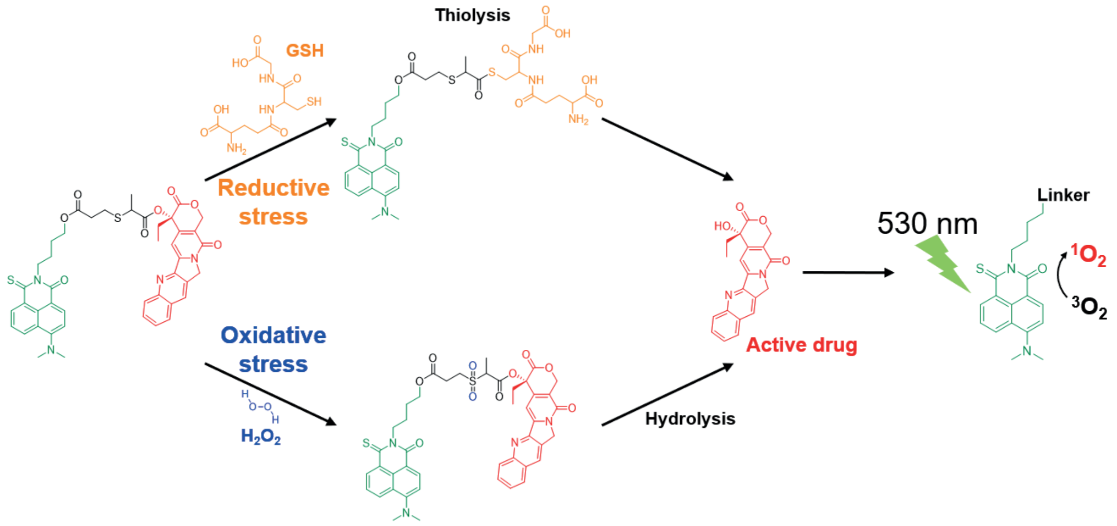
Poster Presentation : **ORGN.P-348**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Strategy for Photodynamic/Chemo Synergistic Therapy through Combination of Photosensitizer and Prodrug

Seongman Lee, Songyi Lee[1,*]

Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

Photodynamic therapy and chemotherapy are types of cancer treatment. In this study, we designed a photosensitizer (RL) to achieve the synergy of photodynamic and chemotherapy. RL consists of photosensitizer part with high singlet oxygen quantum yield and prodrug part activated by two cancer environment triggers (GSH and H_2O_2). In solution study, it showed the increased fluorescence at 430 nm by releasement of camptothecin(CPT) under redox stress conditions. And it exhibited good singlet oxygen quantum yield ($\Phi_\Delta = 0.46$) under 530 nm LED irradiation. In vitro, we studied its low dark toxicity in CT26 cells (murine colon cancer cell) by MTT assay. And we expect therapeutic synergy of its photodynamic/chemo therapeutic ability in vitro. Thus, we suggest the strategy of photodynamic/chemo synergistic therapy, which can increase the therapeutic effect of cancer cell.



Poster Presentation : **ORGN.P-349**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Design and development of benzimidazole-based fluorescent probe and portable fluorescence spectrometer device for the detection of cysteine in human urine

Gyu Seong Yeom, In-ho Song, Su Jeong Park, Satish Balasaheb Nimse*

Institute of Applied Chemistry and Department of Chemistry, Hallym University, Korea

Measurement of cysteine in urine is crucial for evaluating biological metabolism, monitoring and maintaining the immune system, preventing tissue/DNA damage caused by free radicals, preventing autoimmune diseases, diagnosing disorders such as cystinuria and cancer. Among the various methods, fluorometric detection of cysteine using a fluorescence turn-on probe and a portable fluorescence spectrometer device is highly sensitive, simple, rapid, and inexpensive. Herein, we present the synthesis, application of a benzimidazole-based fluorescent probe (ABIA), and the design and development portable fluorescence spectrometer device (CysDDev) for detecting cysteine in simulated human urine. ABIA showed excellent selectivity and sensitivity in detecting cysteine over homocysteine, glutathione, and other amino acids with a response time of a mere 1 min and demonstrated a detection limit of 16.3 nM using the developed CysDDev. Further, ABIA also demonstrated its utility in detecting intracellular cysteine, making it an excellent probe for bio-imaging assay.

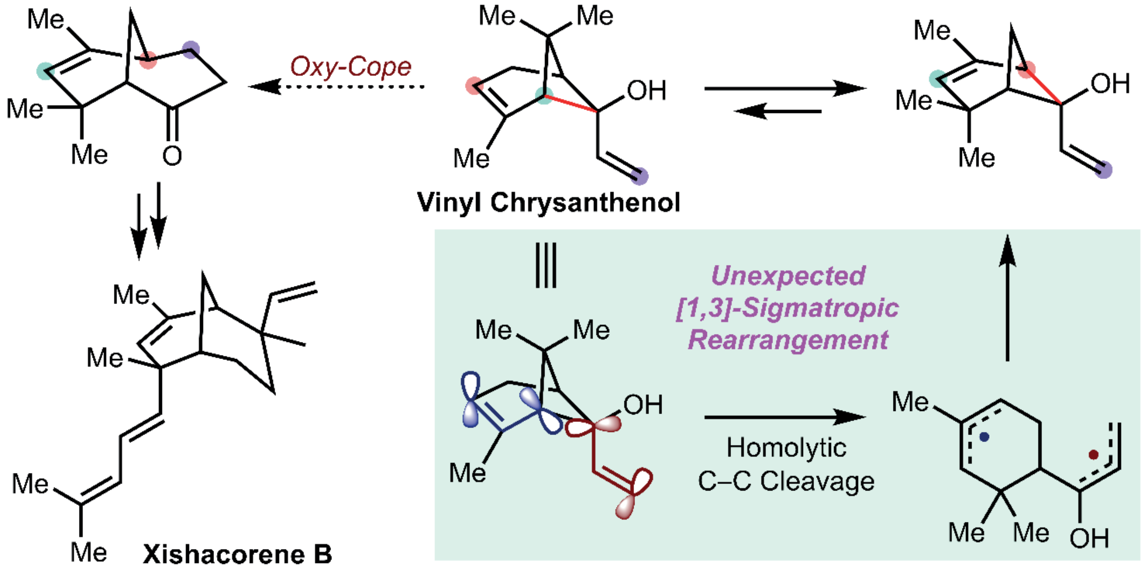
Poster Presentation : **ORGN.P-350**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Understanding [1,3]- and [3,3]-Sigmatropic Rearrangement of Chrysanthenol Core Toward the Synthesis of Xishacorene B

Bohyun Park, Kerry E. Jones[1], Nicolle A. Doering[1], Richmond Sarpong[1,*], Mu-Hyun Baik[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Department of Chemistry, University of California, Berkeley, United States*

Cyclobutanol skeleton has been widely used as a synthetic platform due to its highly strained structure and thus weak C–C bonds. To utilize the cyclobutanol moiety for the synthesis of xishacorene B, we made a vinylchrysanthenol by a 1,2-addition of vinyl magnesium bromide to the chrysanthenone. Against our expectation that the vinylchrysanthenol might undergo an oxy-Cope rearrangement to form a [3.3.1] bicycle, it did not undergo an oxy-Cope rearrangement but an unexpected formal [1,3]-sigmatropic rearrangement. Herein, we will show the detailed analysis of an unexpected formal [1,3]-sigmatropic rearrangement of chrysanthenol derivatives with various computational and experimental methods. Furthermore, on the basis of our understanding, we will showcase the synthetic strategy for the successful oxy-Cope rearrangement and the synthetic route toward a xishacorene B.


Me
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O
Oxy-Cope
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Vinyl Chrysanthenol
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Xishacorene B
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Me
Unexpected
[1,3]-Sigmatropic
Rearrangement
Homolytic
C–C Cleavage
Me
Me
Me
OH

Poster Presentation : **ORGN.P-351**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

One-pot Synthesis of 2,5-Dimethyl-3,4-diphenylcyclopent-2-en-1-one from 3-Pentanone and Benzaldehyde in Deep Eutectic Solvents

Jeong Seob Byeon, Yeong-Joon Kim*

Department of Chemistry, Chungnam National University, Korea

2,5-Dimethyl-3,4-diphenylcyclopent-2-en-1-one was synthesized from 3-pentanone and benzaldehyde via double aldol condensation and successive Nazarov reaction. Because the well-known metal (Re2(CO)10 and TiCl4) catalyzed reaction has some disadvantage in terms of the cost, air-sensitivity and environmental issues, we developed the new reaction conditions in DESs(deep eutectic solvents) system. Some choline chloride-organic acid based Natural DESs were applied to the reaction and we successfully synthesized 2,5-dimethyl-3,4-diphenylcyclopent-2-en-1-one in a relatively short reaction time using a microwave reactor and we will discuss the acid catalyst effect in DESs on the reactivity.

Poster Presentation : **ORGN.P-352**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Boron-containing Multi-Cyclic Fluorescent Materials : Synthesis and Photophysical properties

Jinyeong Heo, Hyein Jung, Seung Soo Yoon*

Department of Chemistry, Sungkyunkwan University, Korea

Developing efficient fluorescent emitters with high efficiency and narrow-band emission is still challenging for organic light-emitting diodes (OLEDs). Herein, we synthesized three boron-containing multi-cyclic blue fluorescent materials fused with nitrogen, sulfur, and oxygen atoms, respectively. The photophysical properties of these three materials were investigated. Sulfur-fused material (DSBNA-tBu) exhibited deep-blue emission peak at 464 nm with small full-width at half-maximum (FWHM) of 47.5 nm. Additionally, the theoretical calculation revealed that DSBNA-tBu has larger spin-orbit coupling (SOC) values and smaller singlet-triplet splitting (ΔE_{ST}) compared with other two materials. This result suggests that sulfur-fused material can serve as promising emitters with the multi-resonance thermally activated delayed fluorescent property (MR-TADF) for the efficient blue OLEDs.

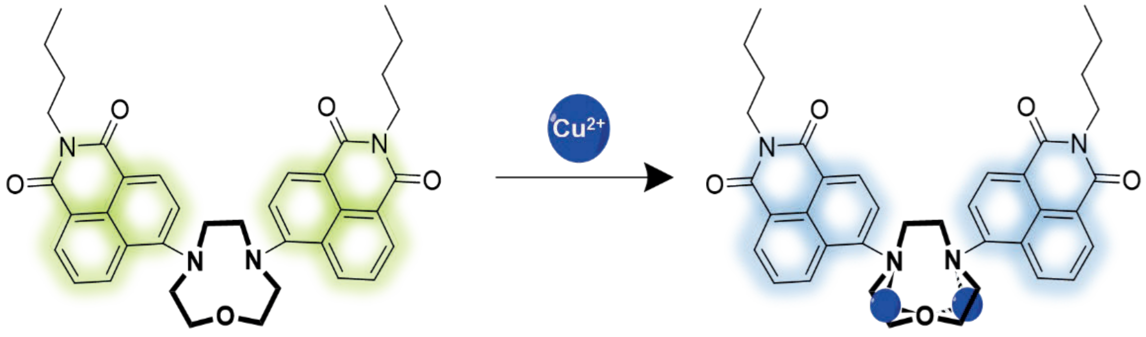
Poster Presentation : **ORGN.P-353**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Development of Intramolecular Charge Transfer Fluorescent Sensor for Cu^{2+} based on Naphthalimide Containing Aza-Crown Ether

Sumin Jeon, Songyi Lee[1,*]

Industry 4.0 Convergence Bionics Engineering, Pukyong National University, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

In humans, copper is an essential metal for the functioning of organs and metabolic processes as a component of several enzymatic systems. However, excessive intake of divalent copper ion (Cu^{2+}) is toxic. Despite the dangers of copper ions, it is important to develop effective methods to detect them as they are one of the common metal contaminants in the environment, widely used in chemical, industrial and agricultural applications. We developed the Intramolecular Charge Transfer (ICT) based chemosensor J2-1 that links 1,8-naphthalimide as a fluorophore and aza-crown ether as a recognition unit to chelate copper(ll) ions. In the J2-1, it can act as an ICT probe by the push-pull effect between the carbonyl group of 1,8-naphthalimide and the aza-crown ether substituted at 4-position. The J2-1 displayed selective and sensitive fluorometric change upon addition of the Cu^{2+}, which was remarkable selective for Cu^{2+} compared to a variety of other metal ions. The J2-1 has green fluorescence at 422 nm, but if the aza-crown ether moiety chelates Cu^{2+}, the push-pull effect decreases, resulting in blue-shifted fluorescence at 312 nm. It was estimated that it interacts with Cu^{2+} through ^1H NMR titraion study.



Poster Presentation : **ORGN.P-354**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

S-Alkylation and N-Alkylation of 2-Mercapto-5-methyl-1,3,4-thiadiazole

Jeong Seob Byeon, Haena Kim, Jaehee Song[1], Yeong-Joon Kim*

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

Heterocyclic compounds have been studied for the application of their derivatives in the pharmaceutical and chemical fields. Thiadizole moiety has been used in a wide range of fields such as pharmaceuticals, agriculture, industry, and dyes. It is known that the alkylation of 2-mercapto-5-methyl-1,3,4-thiadiazole usually goes to S-alkylation in the presence of base catalysts. However, through experiments, it was found that the reaction proceeded without a base, and when the temperature was increased using microwaves, N-alkylation was also observed. The ratio of N-alkylation showed a tendency to increase with increasing temperature. The total yield decreased due to side reactions occurring as the temperature was increased.

Poster Presentation : **ORGN.P-355**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mechanistic Study of Gigantic Porphyrinic Cages Formation Using Mass-Spectrometry

Hochan Lee, Ikjin Kim[1], In-Chul Hwang[2], Kimoon Kim[3,*]

Division of Advanced Material Science, Pohang University of Science and Technology, Korea
[1]*Division of Advanced Materials Science, Pohang University of Science and Technology, Korea*
[2]*Institute for Basic Science, Korea*
[3]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Shape-persistent organic cages or porous organic cages (POCs) have received considerable attention because of their potential use as a versatile functional-materials platform. Formation of their sphere-like structures represents a synthetic puzzle in dynamic covalent chemistry-based self-assembly, and better understanding of the formation mechanism will lead to more controllable and rational design of such cages. Nevertheless, there are only a few mechanistic studies of the cage formation, which deal with only small sized POCs such as [4+4] and [4+6] systems. Recently, we reported the synthesis of porphyrin-based gigantic organic cages ($P_{12}L_{24}$) self-assembled from 12 porphyrins and 24 ditopic linkers without any templates or preorganization. For a deeper understanding of the large cage formation, we have explored the formation mechanism of $P_{12}L_{24}$ using MALDI mass spectrometry. The details of this study will be presented.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **ORGN.P-356**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Audible Sound Controlled Pattern Generation in Blue Bottle Experiment

Ilbong Lee, Ilha Hwang[1,*], Kimoon Kim[*]

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

The blue bottle reaction and its analogues are widely used in chemical demonstrations because of their visual appeal and simplicity. The reaction solution consists of a colored redox-active dye, glucose, and a base. As a well-known example, methylene blue is reduced while glucose is oxidized in a basic condition and consequently loses its blue color. Studies have shown that colored patterns are formed in the solution through convection induced by chemical reactions. Recently, we have demonstrated the use of audible sound to control chemical reactions in a spatiotemporal manner. Sound-induced vibrations of a liquid allows us to control the convection of the fluids and consequently the chemical reactions. In this presentation, we will demonstrate a novel method to generate colored patterns in the blue bottle reaction by applying audible sound. The shape of the resulting pattern is determined by the frequency and amplitude of the applied sound. This study provides a better understanding of the blue bottle reaction and opens new perspectives on the spatiotemporal regulation of chemical reactions using audible sound.

Poster Presentation : **ORGN.P-357**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A fluorescent hybrid complex with a dipolar fluorophore, peptide and serum albumin: Visualization of human glioblastoma

Jong Min An, Dokyoung Kim[1,*]

Biomedical Science, Kyung Hee University, Korea
[1]College of Medicine, Kyung Hee University, Korea

The precise surgery for the pathologic site (i.e. glioblastoma; GBM) determines the prognosis of the patient. Thus, many studies were explored to be more precise surgery. In this vein, fluorescent probes such as fluorescein, Indocyanine green, and 5-ALA, were developed and commercialized to use in the operating room for a trace of GBM. However, they have shown several disadvantages; 1) insufficient selectivity for tumor site, 2) low resolution by photobleaching, 3) blood-brain-barrier disruption by administration of the high dose. To overcome these shortages, for the first time, we designed a GBM-targetable complex consisting of oxazepine fluorophore (OXN-1), tetra-peptide (Ser-Ile-Trp-Val; SIWV), and bovine serum albumin (BSA). To make a hybrid complex, the oxazepine fluorophore was functionalized by the addition of azide moiety (OXN-N3). After copper-catalyzed click chemistry between the azide moiety and alkyne bearing SIWV peptide, the GBM-homing ability was generated (OXN-SIWV). To enhance the targeting ability and biocompatibility, we tried to form the hybrid complex (BSA-OXN-SIWV) using BSA, of which plasma protein is one. The formation of OXN-1, OXN-N3, and OXN-SIWV was identified by using NMR and LC-MS, and the BSA-OXN-SIWV complex was delicately investigated by computing calculation and experimental analysis. The BSA-OXN-SIWV complex showed great performance in terms of GBM-visualization with high selectivity, resolution, photostability, and sufficient biocompatibility. In particular, as the form like a spray, BSA-OXN-SIWV complex could apply in imaging of GBM biopsy derived humans with a negligible background. We strongly believed that the potential of this interesting finding has enough competitiveness to be a clinical tool, compared with approved probes.

Poster Presentation : **ORGN.P-358**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Control of Cascade Reactions via Audible Sound Induced Transient Membraneless Compartments

Tanwistha Ghosh, Hong-guen Lee[1], Ilha Hwang[*], Kimoon Kim[2,*]

Center for Self-assembly and Complexity, Institute for Basic Science, Korea
[1]*Department of Advanced Material Science, Pohang University of Science and Technology, Korea*
[2]*Department of Chemistry, Pohang University of Science and Technology, Korea*

Spatiotemporal control of cascade reactions inside the cell is one of the key steps to regulate important cellular processes in living organisms. To mimic such behavior, scientists have developed several strategies for cell-like compartmentalization such as vesicles, polymersomes, coacervates, etc. Although a considerable amount of progress has been made, one still needs to develop alternative strategies for controlling cascade reactions within spatiotemporally controlled compartmentalized environments in a solution. Herein we present the utilization of audible sound induced liquid vibrations for the generation of transient membraneless compartments within a solution and its utilization for the control of cascade chemical reactions in a spatiotemporal fashion. This approach gives us access to highly reproducible spatiotemporal chemical gradients and patterns, *in situ* growth and aggregation of nanoparticles at predetermined locations or domains formed in a solution. In addition, the application of the nanoparticle patterns for selective cell growth will be presented.

Poster Presentation : **ORGN.P-359**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Audible Sound-driven Transient Segregation and Patterning of Functional Supramolecular Aggregates

Shovan kumar Sen, Seoyeon Choi[1], Ilha Hwang[2,*], Kimoon Kim[3,*]

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

Spatiotemporal control over the formation of multicomponent functional supramolecular polymers in solution is one of the key challenges in front of chemists. These non-covalent supramolecular polymers exhibit different functions such as fluorescence, chirality, etc., which if segregated in the solution may lead to the exploration of novel materials with unanticipated properties. So far various external stimuli such as light, magnetic field, heat, ultrasonic sound, etc., have been used in this direction. The use of audible sound is one of the latest and exciting strategies to control the fate of supramolecular polymers in solution, which operate out-of-equilibrium. Here, we have used audible sound as a guiding stimulus to enable the dissolution of atmospheric O_2 in water, which helps in the spatiotemporal segregation of different functional redox-responsive supramolecular aggregates in water. Using this approach, we demonstrated the transient segregation between homopolymers, heteropolymer, etc. As a proof-of-concept application of segregation of functional supramolecular aggregates, we showed the transient segregation between chiral and achiral supramolecular aggregates as well as two oppositely chiral redox-responsive helical supramolecular polymers. This study may expand the scope of the application of audible sound to gain spatiotemporal control over the functions of supramolecular polymers in solution.

Poster Presentation : **ORGN.P-360**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

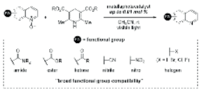
Highly Chemoselective Deoxygenation of Amine *N*-Oxides Using Hantzsch Esters as Mild Reducing

Juhyeon An, Jun Hee Lee[1,*]

Dongguk University, Korea

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

Herein, we disclose a highly chemoselective room-temperature deoxygenation method applicable to various functionalized N-heterocyclic *N*-oxides via visible light-mediated metallaphotoredox catalysis using Hantzsch esters as the sole stoichiometric reductant. Despite the feasibility of catalyst-free conditions, most of these deoxygenations can be completed within a few minutes using only a tiny amount of a catalyst. This technology also allows for multigram-scale reactions even with an extremely low catalyst loading of 0.01 mol %. The scope of this scalable and operationally convenient protocol encompasses a wide range of functional groups, such as amides, carbamates, esters, ketones, nitrile groups, nitro groups, and halogens, which provide access to the corresponding deoxygenated N-heterocycles in good to excellent yields (an average of an 86.8% yield for a total of 45 examples).


FG
RO2C
CO2R
Me
N
H
Me
N
O⁻
metallaphotocatalyst
up to 0.01 mol %
CH3CN, rt
visible light
FG = functional group
NR2
OR
R
CN
NO2
X
(X = I, Br, Cl, F)
amide
ester
ketone
nitrile
nitro
halogen
"broad functional group compatibility"

Poster Presentation : **ORGN.P-361**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

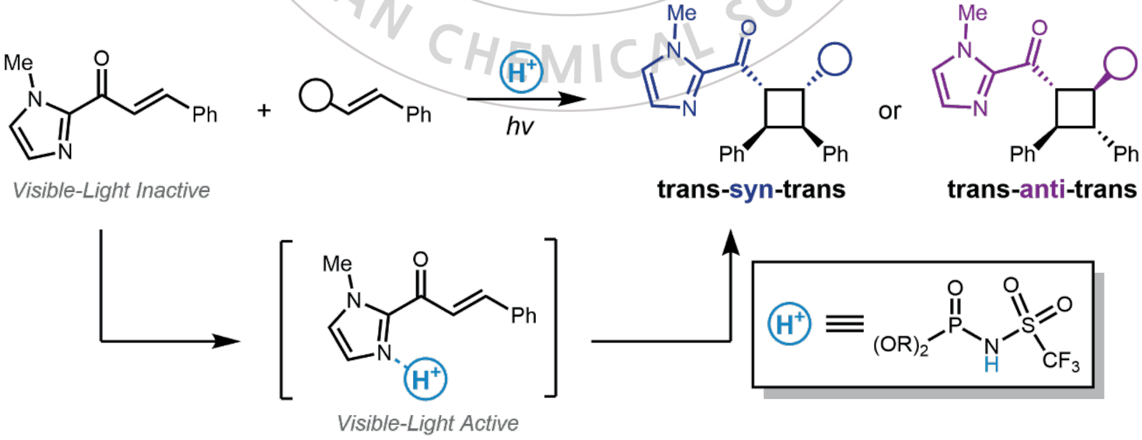
Mechanistic Investigation of Brønsted-Acid Catalyzed Diastereoselective [2 + 2] Photocycloadditions

Hyoju Choi, Bohyun Park, Matthew J. Genzink[1], Tehshik P. Yoon[1,*], Mu-Hyun Baik[*]

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

[1]*Department of Chemistry, University of Wisconsin–Madison, United States*

Photochemical [2 + 2] cycloaddition reactions have been actively studied due to its relatively mild reaction conditions and its highly reactive cyclobutane core as a valuable synthetic platform. Recently, our group and Yoon group has actively studied stereoselective Brønsted-acid-catalyzed [2 + 2] cycloadditions without photosensitizers. We have found that the stereochemistry of the products are highly dependent on the coupling partners and existence of the acid catalysts. More specifically, the addition of the acid in particular couplings totally reverses the stereoselectivity of the products. To reveal the full reaction mechanism and the key factors at the stereo-determining step, detailed mechanistic study by density functional theory calculations and experimental methods is ongoing.



Poster Presentation : **ORGN.P-362**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Structural modulation of short peptides by hydrazone photoswitches

Myeongsu Jeong, Kwonjung Lee, Sangdoo Ahn[1,*], Sunbum Kwon[1,*]

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

Light is a unique stimulus that gives access to non-invasive control of molecules with high spatiotemporal precision. Various families of photoswitches based on *E*/*Z* configurational isomerization or ring opening/closure have been developed and exploited in applications such as dye-sensitized solar cells, information storage, photochromic materials, and synthetic molecular machines. Especially, incorporation of photoswitches into the biomolecules has been of great interest since it allows remote control of their bioactivities in physiological condition. Photoswitches that undergo light-driven *E*/*Z* isomerization (e.g. azobenzenes, stilbenes, indigo derivatives, and fumaramides) have been highlighted in this regard, because their photoisomerization process leads to the drastic change in the overall molecular shape and bioactivity. However, several photoswitching properties, such as excitation wavelength, quantum yield, thermal half-life, resistance to photodegradation, should be carefully optimized for high-fidelity performance of the switching molecules. Recently, hydrazone-based molecular switches that undergo photodriven *E*/*Z* isomerization about the C=N bond have been reported. Of particular note is that some of them have superb properties, such as high photostationary state, good quantum yield, tunable absorption wavelength, fatigue resistance, and exceptional thermal stability of the metastable isomer. Based on these precedent studies, we set out to explore the design and synthesis of new hydrazone switches that can induce light-activated switching motion to control the shape of short peptides. Photophysical properties and isomerization kinetics of the hydrazone switches have been thoroughly investigated, and interestingly, extremely long half-lives of the metastable isomers were well-retained. Moreover, light-activated structural modulation of short peptides has also been demonstrated successfully. We anticipate that the hydrazone photoswitches would constitute a prestigious class of biomolecular modulator with superior switching properties for future bioapplications.

Poster Presentation : **ORGN.P-363**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

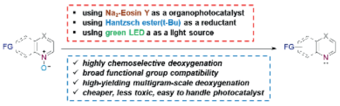
Highly Chemoselective Deoxygenation of N-Heterocyclic *N*-Oxides Under Transition Metal-Free Conditions

Sehyun Kim, Ju Hyeon An, Jun Hee Lee[1,*]

Dongguk University, Korea

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

Because their site-selective C–H functionalizations are now considered one of the most useful tools for synthesizing various N-heterocyclic compounds, the highly chemoselective deoxygenation of densely functionalized N-heterocyclic N-oxides has received much attention from the synthetic chemistry community. We have developed a protocol for the highly chemoselective deoxygenation of various functionalized *N*-oxides under visible light-mediated photoredox conditions with Na_2-eosin Y as an organophotocatalyst. Mechanistic studies imply that the excited state of the organophotocatalyst is reductively quenched by Hantzsch esters. This operationally simple technique tolerates a wide range of functional groups and allows high-yield, multigram-scale deoxygenation.



Poster Presentation : **ORGN.P-364**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Diversification of quinazoline derivatives by microwave-assisted coupling reactions.

Jeong Eun Park, Jeong Seob Byeon, Eul Kgun Yum*

Department of Chemistry, Chungnam National University, Korea

The quinazoline derivatives have attracted intensive interests for drug discovery due to diverse biologically activities such as anti-HIV, anticancer, antimalarial, and anti-inflammatory. In this report, we will discuss microwave-assisted N-Arylation and cross-coupling conditions to diverse haloquinazoline moiety. The green synthetic methods provided fast reaction time, high yields of product, and reducing waste chemicals. The diversified quinazoline moiety could be useful substances for biologically activities screening.

Poster Presentation : **ORGN.P-365**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

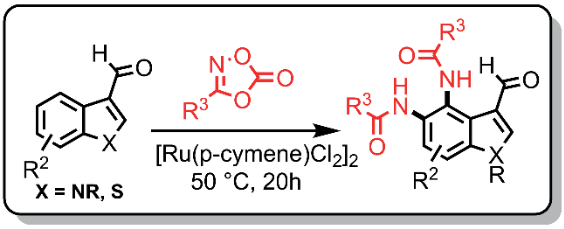
Mechanistic Study of Ruthenium(ll)-Catalyzed Regioselective C4- and C5-diamidation of Indoles

Seok Yeol Yoo, Mu-Hyun Baik*, Yong Rok Lee[1],*

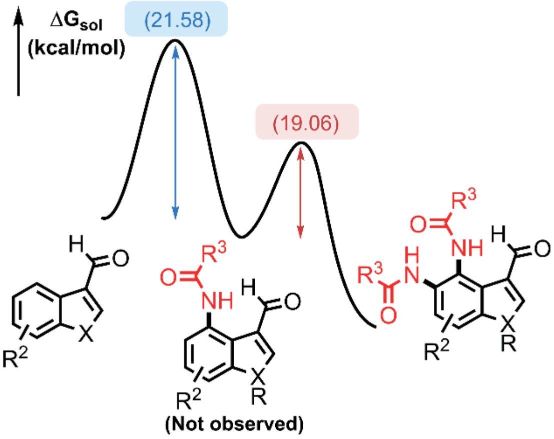
Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

[1]Division of Chemical Engineering, Yeungnam University, Korea

Indole is one of the most important scaffolds in pharmaceuticals and natural products as an aromatic N-heterocyclic compound. Because of this importance, functionalizations of indoles, especially alkenylation and alkylation reactions have been widely studied. Despite the efforts, the amidation by utilizing dioxazolone is still elusive except the cobalt-catalyzed C2-amidation by Wang group.[1]Herein, we demonstrate the direct ruthenium-catalyzed diamidation on C4- and C5- carbon indole derivatives and its mechanism.[2] Density functional theory calculations were used to investigate the origin of selective diamidation. Specifically, the More O’Ferrall-Jencks plot explains the C4-selectivity over the most protic C2-sites by showing that our system follows an electrophilic concerted-metalation-deprotonation pathway. Furthermore, we have shown the detailed mechanism where the implemented amide enables the cascade C5-amidation. The energy barrier and the natural charge analysis were used to explain the observed diamidation product.



- **DFT calculations**
- **Origin of the cascade amidation**



Poster Presentation : **ORGN.P-366**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Control of Chemoselectivity of SET-Promoted Photoaddition Reactions of Fullerene C_{60} with α-Trimethylsilyl Group-Containing *N*-Alkylglycinates Yielding Aminomethyl-1,2-dihydrofullerenes or Fulleropyrrolidines

Hannara Jang, **Dae won Cho**[1,*]

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

Knowledge about factors that govern chemoselectivity is pivotal to the design of reactions that are utilized to produce complex organic substances. In the current study, single-electron transfer (SET)-promoted photoaddition reactions of fullerene C_{60} with both trimethylsilyl and various alkyl group-containing glycinates and ethyl *N*-alkyl-*N*-((trimethylsilyl)methyl)glycinates were explored to evaluate how the nature of *N*-alkyl substituents of glycinate substrates and reaction conditions govern the chemoselectivity of reaction pathways followed. The results showed that photoreactions of C_{60} with glycinates, performed in deoxygenated conditions, produced aminomethyl-1,2-dihydrofullerenes efficiently through a pathway involving the addition of α-amino radical intermediates that are generated by sequential SET-solvent-assisted desilylation of glycinate substrates to C_{60}. Under oxygenated conditions, photoreactions of glycinate substrates, except N-benzyl-substituted analogues, did not take place efficiently owing to quenching of $^3C_{60}{}^*$ by oxygen. Interestingly, *N*-benzyl-substituted glycinates did react under these conditions to form fulleropyrrolidines through a pathway involving 1,3-dipolar cycloaddition of in situ formed azomethine ylides to C_{60}. The ylide intermediates were formed by regioselective H-atom transfer from glycinates by singlet oxygen. Furthermore, methylene blue (MB)-photosensitized reactions of C_{60} with glycinates under oxygenated conditions took place efficiently to produce fulleropyrrolidines independent of the nature of *N*-alkyl substituents of glycinates.

Poster Presentation : **ORGN.P-367**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Asymmetric amino acid derivative Michael Addition with Dimeric Cinchona-Based Phase Transfer Catalysts

Keepyung Nahm*, Hyunsoo Oh

Department of Chemistry, Yeungnam University, Korea

Benzophenone-linked dimeric Cinchona alkaloid ammonium salt Phase Transfer Catalysts (PTCs) have been developed. In the asymmetric amino acid derivative Michael addition of glycinate Schiff base with acrylonitrile, the m,m-directed PTC showed higher enantiomer excess(%ee) values at a temperature of 0 °C~rt. This is different from the asymmetric alkylation, where p,p-PTC showed higher enatioselectivity

Poster Presentation : **ORGN.P-368**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

1,8-Diazabicyclo[5.4.0]undec-7-ene and $POCl_3$ Mediated Reaction of Allyl-protected Amines for Formation of *N*-aryl-substituted Azacycles

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

N-Substituted aryl azacycles are considered as critical building blocks for bioactive molecules including pharmaceuticals, however, synthesis of azacycles is not easily work. Therefore, discovering innovative techniques for the synthesis of *N*-substituted aryl azacycles has been one of the interests of organic chemists. In several previous researchs, many primary arylamines were employed to generate *N*-substituted aryl azacycles directly, restricting the reaction scope. In the multiple-step synthesis, amine groups were commonly protected by allyl groups. Thus, the directly transforming of allyl-protected arylamines to target molecules such as *N*-substituted aryl azacycles is an effective approach due to reduction of reaction steps, and saving costs. Herein, we reported a unique practical procedure for direct conversion of allyl-protected arylamine compounds to *N*-aryl substituted azacycles in the presence of 1,8-diazabicyclo[5.4.0]undec-7-ene and $POCl_3$. In this study, various allyl-protected arylamines were smoothly treated with five-membered and six-membered cyclic ethers to give the corresponding *N*-aryl substituted azacycle structures in high yield. The new simple synthetic procedure using allyl-protected arylamines will be useful for the preparation of a variety of *N*-aryl substituted azacycles.

Poster Presentation : **ORGN.P-369**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Eugenol derived fluorescence 'turn-on' chemosensor for the nanomolar detection of Zn^{2+} ions in solution and in the live cells

Su Jeong Park, Gyu Seong Yeom, In-ho Song, Satish Balasaheb Nimse*

Institute of Applied Chemistry and Department of Chemistry, Hallym University, Korea

A new Schiff base receptor (E)-N'-(5-allyl-2-hydroxy-3-methoxybenzylidene)furan-2-carbohydrazide (FHE) was synthesized by a multistep reaction involving furan-2-carboxylic acid, hydrazine hydrate, and 5-allyl-2-hydroxy-3-methoxybenzoic acid with 87% yield. FHE demonstrated excellent selectivity and sensitivity towards Zn^{2+} ions in UV–vis absorption spectroscopy and fluorescence spectroscopy experiments. FHE showed weak fluorescence emission at 480 nm (λ_{ex} = 315 nm), presumably due to the C=N bond isomerization in the excited state. Interestingly, upon adding Zn^{2+} to the solution of FHE, a prominent ratiometric fluorescence enhancement was observed at 462 nm (λ_{ex} = 315 nm) with a blue shift of 26 nm. FHE showed high selectivity for Zn^{2+} with a K_a of 3.33×104 M^{-1} and LOD of 24.7 nM. The cell cytotoxicity and cell imaging studies indicated the high applicability of FHE for the detection of intracellular Zn^{2+} ions. These results suggest that the FHE is an excellent chemosensor for detecting Zn^{2+} ions. The quick response, easy-synthesis, and high sensitivity make FHE an ideal sensor for detecting Zn^{2+} ions in a semi-aqueous medium and living cells.

Poster Presentation : **ORGN.P-370**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Direct Transformation of *N*-Boc-protected Amines to Amides via Isocyanate Intermediate

Van Hieu Tran, Hee-Kwon Kim[*]

Department of Nuclear Medicine, Jeonbuk National University, Korea

Amide moiety is one of an essential functional group in nature. Amide structures have contributed to form the structure of proteins, medicinal compounds, and materials. Chemical reactions for the production of amides are one of important transformations in organic chemistry. To avoid generation of undesirable side products from reactions of amines, usually *tert*--butyl carbamate (Boc-carbamate) derivatives were used for give target products in the multiple step synthesis. Thus, direct transformation of *N*-Boc-protected amines to the corresponding amides is an effective synthetic approach to reduce reaction steps, which can decrease both cost and time. Herein, we report a novel direct synthetic procedure for preparation of amides from Boc-carbamate under mild reaction conditions. Specifically, novel one-pot reaction was made up of isocyanate production and treating with Grignard reagent to provide desired amides, and large range of target amide structures was smoothly formed at room temperature at high yields. The novel direct synthesis of amides from *N*-Boc-protected amines at mild condition will be a practical method for the generation of useful compounds containing amide moiety.

Poster Presentation : **ORGN.P-371**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Evaluation of Novel TSPO-Hypoxia Fluorescent Probe for Detection of Glioma Tumor

Van Hieu Tran, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

18 kDa Translocator protein (TSPO) was known as the peripheral benzodiazepine receptor (PBR). TSPO is substantially overexpressed in several cancers as well as activated microglial cells in the central nervous system (CNS). TSPO has been considered as an important biological target for diagnosis and therapy of cancers. Therefore, development of several TSPO ligand-based molecules has been carried out by scientists. Besides, hypoxia is one of properties of many solid tumors. In this study, novel fluorescent compound with TSPO ligand structure and hypoxia sensitive moiety was designed for the detection of Glioma. *N*-(2-Hydroxybenzyl)-*N*-(4-phenoxypyridin-3-yl)acetamide-based TSPO ligand structure was synthesized from 4-chloro-3-nitropyridine, and then it was conjugated with a 2-nitroimidazole derivative, a hypoxia sensitive structure, by amide linkages in mild conditions. Subsequently, SCy5.5 was attached to the combined TSPO-Hypoxia structure. Next the novel TSPO-hypoxia fluorescent compound was used to conduct *in vivo* and *ex vivo* animal imaging study using glioma bearing mice. The results showed that the novel TSPO-hypoxia fluorescent compound highly accumulated in the Glioma tumor location. The animal study suggests that novel TSPO-Hypoxia fluorescent probe can be a promising imaging agent for detection of glioma cancer.

Poster Presentation : **ORGN.P-372**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Highly efficient Synthesis of Azepane-Derived β-Amino Acid

Ingyu Han, Soo Hyuk Choi[1,*]

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

Cyclic β-amino acids are a useful monomer in rigidifying and stabilizing the secondary structure of peptide oligomers. ACPC, ACHC, ACHpC are commonly used cyclic β-amino acids that have five to seven-membered ring, but have a problem in applying to biomedicinal study because of there high hydrophobicity. Unlike those cyclic β-amino acids, azepane-derived β-amino acid (cis-4,5-AAZpC) can control it's hydrophilicity as it can easily form acid salt with ring itself. We studied an efficient method to synthesize cis-4,5-AAZpC. With sonication, this reaction can be achieved in a fast and solvent-free way. Using sonication for the reductive amination or synthesis of β-enamino esters was already reported, but using chiral amine to afford β-amino esters with sonication hasn't been examined. In this study, we used chiral (R)-(+)-1-phenylethylamine to get (4S,5R)-AAZpC. By this method, enantiopure (4S,5R)-AAZpC can be obtained with great yields.

Poster Presentation : **ORGN.P-373**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Iridium(NHC)-catalyzed Intramolecular Transfer Hydrogenation using Glycerol Carbonate

Yeon Joo Cheong, Mi-hyun Lee, Hee Min Byeon[1], Hye-Young Jang[2,*]

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

Recently, studies on transition metal-catalyzed transfer hydrogenation (TH) have been actively reported. This is an intermolecular reaction in which hydrogen atom is transferred from H-donors to H-acceptors. However, examples of intramolecular TH have not been reported yet. In this presentation, we report for the first example of Iridium(NHC)-catalyzed intramolecular TH using glycerol carbonate (GC). GCs dissociate into glycerol and carbonate, which act as H-donor and H-acceptor, respectively, under basic conditions. Then, they can go through an intramolecular reaction using efficient catalysts. We synthesized iridium catalysts using a ligand with a flexible structure in which alkyl chains connect three imidazole rings. The catalysts were successfully applied to the reaction with high TONs of formates and lactates. The results and plausible mechanisms will be discussed.

Poster Presentation : **ORGN.P-374**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Complex Effects of Various Terminal Groups on the 12/10-helix Structure of Unnatural β-Peptides

Junyeong Jeong, Soo Hyuk Choi[1,*]

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

In order to study the effect of terminal groups on the helical structure of β-peptides, foldamers based on tetrapeptide backbone were synthesized using 2-aminocyclohexanecarboxylic acid (ACHC), a kind of unnatural β-amino acid, as a monomer. And after introducing various capping groups to each of the *N*- or *C*-terminus of these peptides, the folding structure was analyzed using Circular Dichroism and Single Crystal X-ray Diffraction.Most of the β-peptides composed of only β-amino acids have a 12/10-helix structure, and in the solution phase, the *P*-helix (Right-handed helix) structure and the *M*-helix (Left-handed helix) structure are rapidly interconverted. In this case, depending on which oxygen and hydrogen of the amide groups form hydrogen bonds more strongly, the directionality of the 12/10-helix structure can be strongly induced in a specific direction. And in order to control this effect, the tendency of the helical structure, which has the same backbone, but changes according to which terminal groups are bound, was confirmed.

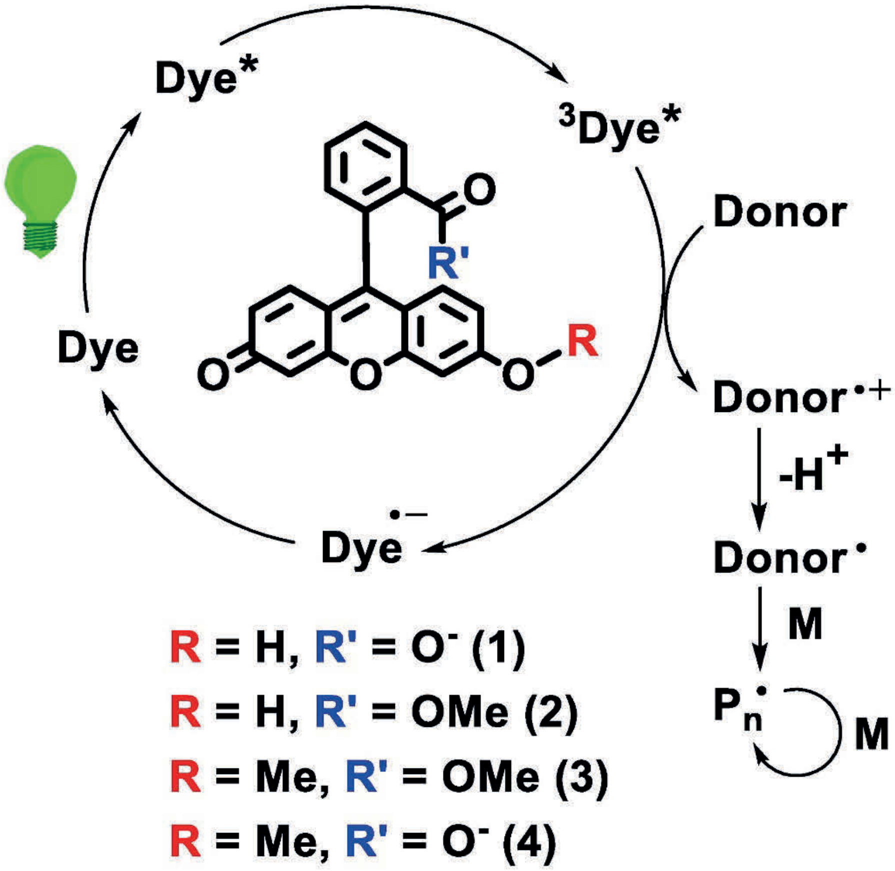
Poster Presentation : **ORGN.P-375**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Photoinitiated Free-Radical Polymerization of Methyl Fluorescein Derivatives under Visible Light

Joseph Nganga, Young Jae Jung[1], JungKyu Lee[2,*]

Chemistry, Kyungpook National University, Congo, Democratic Republic of the
[1]*Chemistry, Kyungpook National University, Korea*
[2]*Department of Chemistry, Kyungpook National University, Korea*

Surface-initiated photopolymerization under visible-light is of great interest nowadays and has a wide range of applications in diverse fields such as sensors, coating, tissue engineering, and dental healing (Jacques Lalevée et al., 2016). Since most of monomers, oligomer or prepolymers are transparent to light, the photocatalyst plays a pivot role during the photopolymerization process and appears to be the most important component (Joanna Ortyl et al., 2021). The design of photocatalysts with better optical properties is therefore a relevant topic of research and in this regard, xanthene dyes are one the best candidates. In this research, we investigate the effect of substituents on the photocatalytic efficiency of xanthene dyes (i.e., methyl ether of fluorescein, methyl ether ester of fluorescein, and methyl ester of fluorescein) using the visible-light initiated photopolymerization. Assuming the optical properties mainly depend on the electronic distribution along the molecule, we speculate that the outcome of our research would bring out useful insights in the design of photocatalysts for photopolymerization.


Dye*
³Dye*
Donor
Donor•+
-H+
Donor•
M
Pn•
M
Dye•−
Dye
R'
R
O
O
O
R = H, R' = O- (1)
R = H, R' = OMe (2)
R = Me, R' = OMe (3)
R = Me, R' = O- (4)

Poster Presentation : **ORGN.P-376**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Imines and Ketones via Palladium-Catalyzed Reverse-Polarity Chemistry

Seungmi Lee, Inji Shin*

Department of Fine Chemistry, Seoul National University of Science & Technology, Korea

Imines and ketones are readily found and important building blocks in synthetic intermediates. We developed a new synthetic method using a concept ‘reverse-polarity’ to prepare a variety of diarylimines and diarylketones. Particularly, acylsilanes and iminosilanes were used as an anion equivalent in palladium-catalyzed cross-coupling reactions. Due to the reactivity of acylsilanes and iminosilanes, diaryliodonium salts were chosen as a coupling partner rather than aryl halides because the reaction with aryl halides did not give the desired product. Diarylimines and diarylketones with electron-neutral, -withdrawing as well as –donating substituents were successfully prepared in excellent to moderate yields after extensive optimizations.

Poster Presentation : **ORGN.P-377**

Organic Chemistry

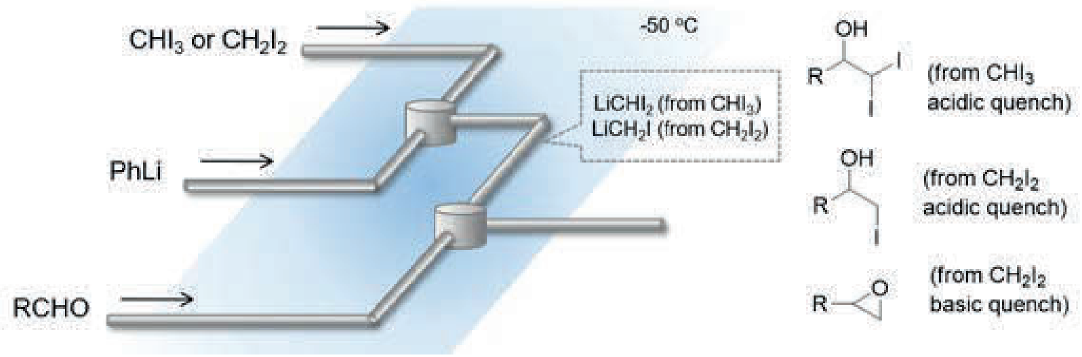
Exhibition Hall 1 FRI 11:00~12:30

Generation and utilization of iodo-containing methyllithiums via continuous-flow system

<u>Nayoung Kim</u>, Hyune-Jea Lee, Heejin Kim*

Department of Chemistry, Korea University, Korea

Organometallic reagents are known as important and commonly utilized tools in organic synthesis. However, Li/Hal carbenoids are among the most reactive species and have difficulty in synthetic applications due to their instability of rapid decomposition to carbene. Herein, we reported that generation of highly unstable diiodomethyllithium and iodomethyllithium was successfully achieved in a continuous flow reactor. Under the optimized condition for generation of carbenoid intermediates in flow, we directly synthesized vicinal halohydrins which are versatile building blocks and key intermediate of many bioactive compounds. Furthermore, epoxide or iodohydrin was selectively obtained depending on the use of an acidic or basic quenching.



Poster Presentation : **ORGN.P-378**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Flow Synthesis of Multi-Substituted Silanes Through Potassium *tert*-Butoxide Catalyzed Reaction of Functional Aryllithiums with Hydrosilanes

Changmo Kwak, Hyune-Jea Lee, Dong Pyo Kim[1,*], Heejin Kim[*]

Department of Chemistry, Korea University, Korea

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

Synthesis of organosilanes as important structural molecules has received substantial attention in the numerous research fields including organic, material and pharmaceutical chemistry. Even if diverse synthetic methods for the formation of carbon-silicon bonds have been reported, a site-specific and atom-economic method for silylation is still highly required. Herein we report a continuous-flow approach to selective and sequential mono-, di-, and tri-functionalizations of un-functionalized hydrosilanes via serial organolithium reactions catalyzed by earth-abundant metal compounds. Especially, the combinatorial functionalizations of trihydrosilane were achieved to provide every imaginable combination of tetra-substituted organosilane libraries based on an accurate reaction control using an integrated one-flow system.

Poster Presentation : **ORGN.P-379**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Development of Selective Electrooxidation methode for Sulfoxide and Sulfone Synthesis using Solvent Effect

Jin Kyu Park, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Sulfoxide- and sulfone-containing derivatives are widely utilized in various applications, such as pharmaceutical and agrochemical manufacture, catalysis, and materials chemistry. A variety of synthetic methods for the preparation of sulfoxides and sulfones have been developed to date. Among them, most of the methods using an oxidizing agent are well known. However, we developed a synthetic method using electrochemistry, which is an eco-friendly method. Sulfoxides are selectively obtained in good yield under a constant current of 5 mA for 10 h in DMF, while sulfones are formed as the major product under a constant current of 10 or 20 mA for 10 h in MeOH. Through a control experiment, we found that The oxygen of both the sulfoxide and sulfone function is derived from water.

Poster Presentation : **ORGN.P-380**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of beta-ketonitriles via the condensation of amide and acetonitrile

Myeong Seong Park, Jonghoon Oh*, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Beta-ketonitriles is one of the most valuable functionality in organic synthesis because it can readily be converted a variety of heterocyclic compounds. Various synthetic methods for beta-ketonitrile have been developed. Among them, transiton-metal catalyzed carbonylative coupling, electrophilic cyanation, and acyl substitution reaction are straightforward and most often employed tools for the preparation of beta-ketonitrile. However, there is no report of the acyl substitution reaction of amides. Herein we report the synthesis of beta-ketonitrile from the reaction of amides and acetonitrile. We found that N-phenyl-N-tosyl benzamides reacted with acetonitrile in the presence of LiHMDS, the corresponding benzoylacetonitriles were formed in good yields.

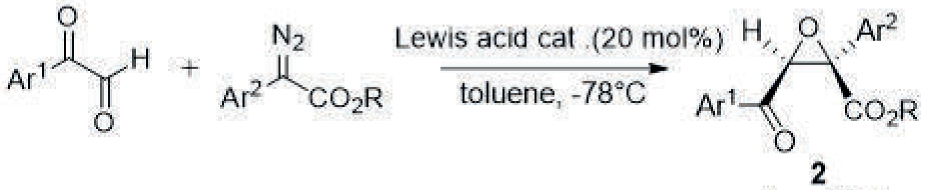
Poster Presentation : **ORGN.P-381**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Enantioselective Epoxidation of Aldehyde with Aryl Diazo Ester: Synthesis of Chiral Tri-Substituted Epoxide

Dong Guk Nam, Hye-Min Jeong, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Optically active α, β epoxy ketones are the most versatile structures in organic synthesis. The ketone and epoxide moiety can be functionalized to produce various intermediates for the synthesis of biologically active molecules. An enantioselective synthesis of tri-substituted α, β epoxy ketones has been developed with aryl aldehyde and aryl diazo ester in the presence of Lewis acid catalyst. This methodology was performed and produced chiral tri-substituted α, β epoxy ketones with excellent ee (up to 99% ee) and high trans/cis ratio (1:>20) in excellent yield (up to 99%). Chemical transformation of chiral tri-substituted epoxide was conducted to demonstrated synthetic utility of methodology.



2
d.r. >20:1
up to 99% yield
up to 99% ee

Poster Presentation : **ORGN.P-382**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Cysteine-Fluorescent Probe for Visualization of Glioblastoma

Youngwoong Kim, **Dokyoung Kim**[1,*]

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

A fluorescent probe has been recognized as a clinical tool due to its selectivity, sensitivity, and intuition toward targets. Especially, when precise resection for glioblastoma (GBM) as one of brain cancer, many fluorescent probes (e.g. indocyanine green) was approved to use in GBM surgery. Despite their utilities, the unfocusing ability for GBM makes the GBM-patients suffer a poor prognosis after surgery. To address these issues, GBM-responsive probes have been stood out. Cysteine (cys) is one of the thiol group-containing sulfur (-SH) in a biological system. Although cys has the potential of a biomarker for GBM, its similarity to homocysteine (hcy) makes the cys-detection of fluorescent probe more difficult. Herein, we introduce a new approach to detect cys with high specificity and selectivity. [Ref: 1] We controlled the electron-density at an aromatic ring of nitrobenzoxadiazole derivates (NPO-series); 1) Electron-normal aromatic ring (NPO-A), 2) Electron-deficient aromatic ring with pentafluorine (NPO-B), 3) Electron-rich aromatic ring with p-methoxy (NPO-C). Interestingly, electron-density could regulate the cys-responsive rate, following that NPO-B with an electron-deficient group showed the selectivity and sensitivity for cysteine. The formation of NPO-series was identified by NMR and MS. Besides, we confirmed the in human-GBM cells, in GBM-xenograft, and ex vivo (GBM-xenograft and human biopsy) for cysteine detection of NPO-B. As a result, NPO-B classified between normal site and GBM site fastly (time: 30 min) as well as NPO-B did not show immune toxicity in mice when administered. Based on promising works of NPO-B for cys, we believed that NPO-B could propose not only an ideal approach related cys detection and visualization of GBM in the clinical field.

Poster Presentation : **ORGN.P-383**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Enantioselective Friedel-Craft Reaction of Hetero-aryl Compounds with *ortho*-Quinone Methide.

Yoon Sung Cho, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

One of the strongest synthetic method to accomplish carbon-carbon bond was Friedel-Crafts reaction with aromatic compounds. Throughout Friedel-Crafts reaction with aromatic compounds, we can synthesize the triarylmethanes (TRAMs) that contain the central sp^3-hydridized carbon atom with three aryl groups. Our group reported the highly enantioselective Friedel-Crafts reaction, produced the triarylmethanes (TRAMs), of various furans with *ortho*-quinone methides in the presence of Lewis acid catalyst. Especially, *ortho*-quinone methides could be intermediates that great electrophiles for Friedel-Crafts reaction with various furans. This methodology produced the triarylmethanes (TRAMs) in excellent yield with excellent enantioselectivity. (up to >99%). Thus, chemical transformation of the triarylmethanes (TRAMs), including unsubstituted furans, conducted to demonstrated synthetic utility of methodology and offer the possibility the various applications.

Poster Presentation : **ORGN.P-384**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Visible-Light Initiated Enantioselective Addition of *α*-Aminoalkyl Radical to *α*, *β*-Unsaturated Carbonyl Compounds

Yea Suel Lee, Do Hyun Ryu[1,*]

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

Electron donor-acceptor (EDA) complex, which is an association of electron donor and electron acceptor in the ground state, has been extensively studied since the initial studies of Mulliken in 1950. The EDA complex has recognized as an attractive synthetic method because this complex can generate radical species under mild reaction conditions by light irradiation and does not require any additional photosensitizer. However, to the best of our knowledge, chiral Lewis acid-assisted EDA complex to initiate catalytic asymmetric radical reaction has not been reported. Herein, we successfully developed the first example of visible-light induced enantioselective radical reaction to *α*, *β*-unsaturated carbonyl compounds using ternary EDA complex in the presence of chiral oxazaborolidinium ion as a chiral Lewis acid catalyst. With this EDA complex induced radical reaction, we synthesized optically active *β*-amino alcohol derivatives with high yields (up to 93%) and high enantioselectivities (up to 95% ee). Furthermore, we successfully applied this synthetic methodology to *α*, *β*-unsaturated ketones. Compared to the acroleins, *α*, *β*-unsaturated ketones afforded 1,4-addition products with high yields (up to 99%) and high enantioselectivities (up to 94% ee).

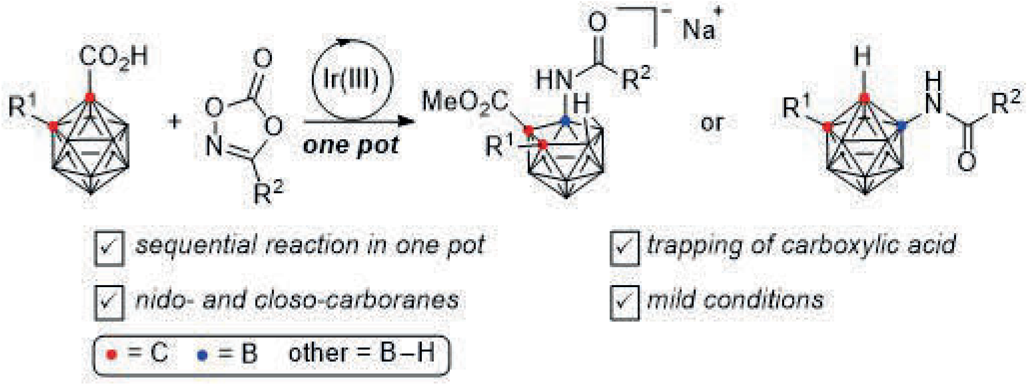
Poster Presentation : **ORGN.P-385**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Iridium(III)-Catalyzed Cage B(4)-Amidation Reaction of *o*-Carboranes with Dioxazolones: Selective Synthesis of Amidated *o*-Carboranes and Amidated and Methoxycarbonylated *nido*-Carboranes

Kyungsup Lee, Gi Uk Han, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Carboranes, which are recognized as a type of three-dimensional kindred form of benzene, have found a number of applications in boron neutron capture therapy (BNCT) as medication, in organometallic and coordination chemistry as novel ligands, and in supramolecular design and materials as building blocks. However, the distinctive structures of carboranes make their derivatization laborious, which results in a restricted application range. Therefore, it is highly required to develop new synthetic methods for the functionalization of carboranes. Described is the Ir-catalyzed cage B(4)-amidation of *o*-carboranes with dioxazolones by carboxylic acid-assisted B(4)−H bond activation under mild conditions, affording amidated *o*-carboranes and amidated and methoxycarbonylated *nido*-carboranes through sequential B(4)-amidation, *O*-methylation, and B(3)-deboronation in one pot. Carboxylic acid used as a directing group after the cage B(4)-amidation is efficiently trapped by $TMSCHN_2$ instead of undergoing decarboxylation. Mechanism studies demonstrated that the *O*-methylation through trapping of acid occurred first, followed by the B(3)-deboronation.



Poster Presentation : **ORGN.P-386**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Vinyl Sulfone Synthesis via Three-Component Copper-Catalyzed Decarboxylative Addition

An Seunghwan, Sunwoo Lee*, Jonghoon Oh*

Department of Chemistry, Chonnam National University, Korea

The synthesis of vinyl sulfone derivatives via the reaction of arylpropiolic acids, K2S2O5, and aryl boronic acids is reported. The CuBr2/1,10-phenanthroline catalytic system in the presence of acetic acid provides the desired vinyl sulfones in moderate to good yield.

Poster Presentation : **ORGN.P-387**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Rational design and Synthesis of a Near-infrared Probe for In Situ Imaging of OGA

Chaeyeong Lee, Ahmed A. Elbatrawy[1], Jongseung Kim[2], Ghilsoo Nam[3,*]

Chemistry, Korea University, Korea
[1]*Division of Bio-Med, University of Science & Technology, Korea*
[2]*Department of Chemistry, Korea University, Korea*
[3]*Center for Neuro-Medicine Brain Science Institute, Korea Institute of Science and Technology, Korea*

O-GlcNAcylation is a ubiquitous glycosidic addition of O-linked N-acetylglucosamine (O-GlcNAc) to nucleocytoplasmic proteins. Unlike phosphorylation, this post-translational protein modification is principally governed by two enzymes; O-GlcNAc transferase (OGT), which couples O-GlcNAc to the acceptor protein; and O-GlcNAcase (OGA) that hydrolyses this action. Irregular levels of O-GlcNAc are physiologically associated with numerous pathogenesis such as cancer and neurodegeneration. Therefore, there is an urgent demand to understand O-GlcNAcylation at levels of molecular biology and enzyme regulation. While many fluorescent probes were designed to detect OGT, only few fluorophores were synthesized to monitor OGA intracellularly. In the present work, we rationally designed a near-infrared (NIR) small molecule probe (OGA-1) for in situ visualization of OGA. We expected that OGA-1 could serve as a cost-effective sensor for tracking OGA under both ex vivo and in vivo experiments.

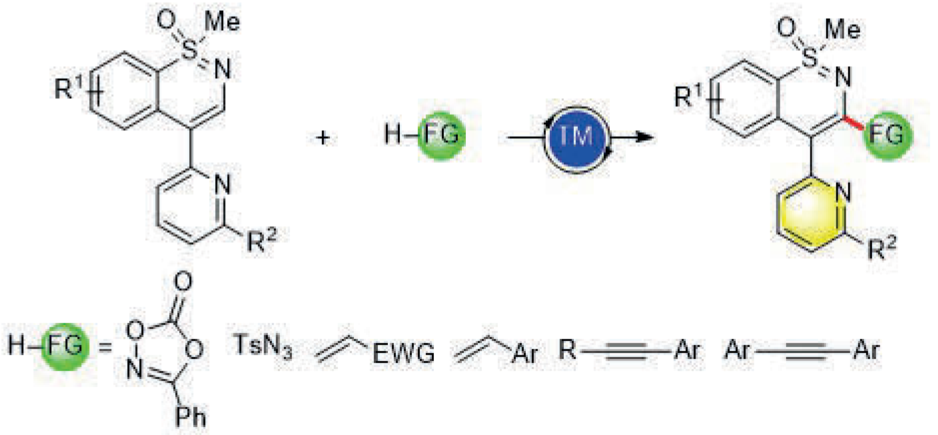
Poster Presentation : **ORGN.P-388**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of 3,4-Functionalized Benzothiazines through C−H Activation

Hee Chan Noh, Chanyoung Maeng, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Sulfoximines are important structural motifs that have been applied as pharmaceuticals, bioactive compounds, and agrochemicals. Among the numerous sulfoximine derivatives, 1,2-benzothiazines are more attractive pharmacophores as a type of cyclic sulfoximine. As a consequence, the development of novel synthetic methods for the construction of cyclic sulfoximines and their functionalization are highly needed. Herein we introduce method for the synthesis of a wide range of 1,2-benzothiazines bearing pyridyl, amide, sulfonamide, alkenyl, as well as aryl groups in 3,4-position has been developed using transition metal-catalyzed C−H activation reactions of pyridylbenzothiazines with dioxazolones, tosyl azide, alkenes, alkynes, and diaryliodonium salts. The present reaction provides an efficient method for the synthesis of a variety of 3,4-functionalized benzothiazines from readily available starting materials and benefits a broad substrate scope, high functional group tolerance, and good regioselectivity.



☑ challenging products
☑ new scaffolds
☑ 3,4-functionalized 1,2-benzothiazines
☑ regioselective
☑ broad substrate scope
☑ wide functional group tolerance

Poster Presentation : **ORGN.P-389**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Investigation and Discovery of Schiff Base Derived Anticancer Prodrug in Biological Imaging and its Target Delivery

Lavanya Gopala, Min Hee Lee[1,*]

Department of Chemistry, Sookmyung Women's University, India
[1]*Department of Chemistry, Sookmyung Women's University, Korea*

Gemcitabine (GMC) is a nucleoside analogue used for an antimetabolite of deoxycytidine to control non-small cell lung, pancreatic, metastatic breast, and recurrent ovarian cancers. Despite the clinical success of GMC, its short plasma half-life and adverse toxicity, such as myelosuppression, greatly limit its chemotherapeutic efficacy. GMC is a non-fluorescent antitumor agent. GMC delivery system in a specific region as well as fluorescence-on, would be valuable for in vivo and vitro use. Theranostics, a special type of drug delivery system with the capability of real time monitoring of drug release, draws attention from medical or pharmaceutical sciences. An endowed theranostic drug delivery system with a targeting unit such as biotin moiety might be an ideal candidate for the target-selective drug delivery system, which has been demonstrated. They can encapsulate both hydrophilic and hydrophobic drugs in their internal water compartment and lipid membrane, respectively. The main characteristics of these systems include biocompatibility, small size, low toxicity, low clearance rate, controlled release of drugs, and the ability to target cancer tissues. In other interesting studies, a series of lipophilic conjugates of GMC were prepared by conjugating the N4 -amino moiety of GMC with different linear acyl chains, i.e., stearoyl, heptanoyl, lauroyl and valeroyl acyl chains and the prodrugs were incorporated into liposomes. Encapsulation of the synthesized prodrugs of GMC in liposome formulation supported the drug from degradation, assuring intracellular release and long plasma half-life of the parent drug. On the other hand fluorescence-based imaging for monitoring cellular uptake and prodrug activation processes. They also need to provide a read-out that can be monitored readily under the conditions typical of cellular analysis. This makes fluorescent probes of particular interest. To construct pH-responsive and drug-containing DNA structures for facilitating the intracellular nuclease mediated drug release and enhancing their anticancer efficacy. Therefore, we view an ability to effect, the addition of gemcitabine would lead to the formation of Schiff

base, conjugates of fluorescent probe linked–Gemcitabine system as a tumour specific theranostic anticancer prodrug.

Poster Presentation : **ORGN.P-390**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Flow-Assisted Green Synthesis of [6,4]CPPy through Serial Microreactions

Yongju Jeon, Hyune-Jea Lee[1], Heejin Kim[1,*]

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

The synthesis of 2,2'-bipyridine embedded CPP(CPPy) ligand has illustrated a general strategy for coordinating the nanoring framework to common metal centers. However, the multi-step conditions and environmentally unsustainable methodology for synthesis of CPPy need to be improved for general access to the CPPy. Herein, we developed straightforward synthesis of [6,4]CPPy in four steps thorugh serial microreactions by using flow microreactors. In this study, 2-MeTHF was used instead of THF or Et2O solvent for organolithium reaction for green synthetic manner. To overcome low reactivity in 2-MeTHF, we searched halogen-lithium exchange reaction conditions using various organolithium reagents. A selective nucleophilic addition of the unprotected p-benzoquinone minimizing the formation of undesired double-added product was successfully achieved in high yield. Moreover, two repeated lithiation step of 1,4-dibromobenzene with sequential reaction of N-L-shaped unit provided N-U-shaped precursor of [6,4]CPPy in the continuous-flow microreactors, which was dimerized and aromatized to synthesize [6,4]CPPy. In addition, nitrogen doped [6,4]CPPy showed red-shifted UV-vis absorption and emission compared to simple [10]CPP.

Poster Presentation : **ORGN.P-391**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

(Iminopyridine)Pd(II)-catalyzed poylmerization of carbon monoxide and olefins

Yongmoon Yang, Hye-Young Jang[1,*]

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

Converting carbon monoxide (CO), which can cause global warming, into high value-added products has environmental and economic merits. Especially, polymerization of CO and ethylene using palladium catalysts produces highly valuable engineering plastic such as polyketones. The Shell's catalyst, commonly used for the synthesis of polyketones, is air/moisture sensitive. In addition, it isn't suitable for introducing aromatic alkenes into the polyketones chain. To solve the low thermal stability and solubility of polyketones, the chemical modification of polyketones by incorporating aromatic alkenes is urgent. In this study, we synthesize the air/moisture stable palladium catalysts involving iminopyridine ligands, which are employed for co- and terpolymerization of CO and olefins, resulting in the modification of properties. By varying *N*-substituents, the steric and electronic effects of ligands were modulated.

Poster Presentation : **ORGN.P-392**

Organic Chemistry

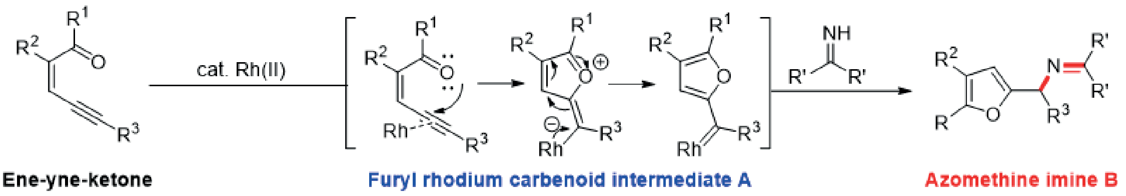
Exhibition Hall 1 FRI 11:00~12:30

Rh(II)-Catalyzed N-H Bond Insertion Using Ene-Yne-Ketones with N-H Imines

<u>Hojun Cho</u>, Juhyun Kim*

Department of Chemistry, Gyeongsang National University, BK21 FOUR, Research Institute of Natural Science, Korea

Selective insertion of X-H (X= C, N, O, Si etc.) bonds through metal carbenoids is an attractive synthetic strategy in terms of high efficiency, atom-economy, and broad reaction scope. In this work, we have developed atom-economical simple method of N-H imine insertion through in-situ generated Rh-carbenoid starting from ene-yne-ketones, affording azomethine imines **B**. In the presence of Rh(II) catalyst, alkyne moiety in ene-yne-ketones was activated, which then underwent 5-exo-dig cyclization to form zwitterionic intermediate **A**, furyl rhodium carbenoid intermediate. Then, N–H imines could subsequently participate in a metal carbene migratory insertion process to give the N–H inserted products, potentially useful in catalytic asymmetric umpolung reactions to access amino acid derivatives and useful chiral amines.



Poster Presentation : **ORGN.P-393**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Efficient synthesis of bicyclic benzoxaphosphole oxide heterocycles via three-component coupling reaction involving arynes, phosphites, and ketones

HeeJin Jeong, Hyo Jae Yoon, Junwon Choi[1,*], Seojung Han[2,*]

Department of Chemistry, Korea University, Korea
[1]*Department of Molecular Science and Technology, Ajou University, Korea*
[2]*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

An efficient and transition-metal free three component reaction with benzynes, obtained in situ from 2-(trimethylsilyl)aryl triflates, phosphites, and ketones was developed to generate bicyclic benzoxaphosphole oxides. We discovered that a variety of functional groups were tolerant under the reaction conditions affording diverse benzoxaphosphole oxides in moderate to good yields. We believe that this reaction could be useful for preparing organophosphorus compounds encountered in natural products, pharmaceutical compounds, and agricultural chemicals.

Poster Presentation : **ORGN.P-394**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Supramolecular Nanomaterial Based on Redox-responsive Intracellular Assembly of Ferrocene-peptides Bioconjugates to Control Cell Fate

Gaeun Park, Ja-Hyoung Ryu*

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

Supramolecular nanomaterials have a critical role in the cell since they interact with cell components and regulate cellular functions in a biological system. Although the nanomaterial is considered a useful tool in biomedical applications, a low delivery efficiency due to protein corona and an immune response is the main challenge. To overcome the drawback, we present a new system to build supramolecular nanomaterials based on the redox-responsive intracellular assembly to control cell fate. Under redox-stimuli, ferrocene moiety exhibits reversible transformation, in which neutral/ hydrophobic ferrocene groups are converted to positive charged/ hydrophilic ferrocenium groups. Due to its redox-reversibility, the ferrocene-peptide conjugates have been used as attractive building blocks for self-assembly and supramolecular nanomaterials with various applications. Here, we propose the intracellular assembly of Fc-FF drives the construction of nanomaterial within the cancer cell, regulates the function of cell components, and controls cell fate. Redox states of ferrocene are turned on in the presence of overexpressed GSH, enabling redox-responsive intracellular assembly, and thus the system to construct nanomaterials operate in the tumor tissue selectively. Accordingly, this study provides a simple tool for building supramolecular nanomaterials in cell and a new possibility for intravenously injected water-soluble therapeutic drugs.

Poster Presentation : **ORGN.P-395**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Microwave-assisted metal-catlyzed diversification of pyrrolo[3,2-d]pyrimidines.

Jeong Seob Byeon, Yeong-Joon Kim*, Eul Kgun Yum

Department of Chemistry, Chungnam National University, Korea

Heterocyclics have attracted particular interest as a moiety for drug design. Almost pyrrolo[3,2-d]pyrimidines have to synthesis for drug discovery research, so we are interesting in establishing chemical library of pyrrolo[3,2-d]pyrimidines for screening drug candidates to various diseases. In this presentation, we will discuss microwave–assisted metal-catalyzed N, O-arylation and diverse metal-catalyzed cross-coupling reactions for facile introduction of different function group to pyrrolo[3,2-d]pyrimidines. Microwave assisted organic synthetic methods showed green chemistry approach for efficient energy saving, better yields of desired products, and fast reaction rates.

Poster Presentation : **ORGN.P-396**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fluorescent probes targeting specific cellular organelle for simultaneous monitoring of viscosity and nitric oxide

Sun Young Park, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Intracellular viscosity is a physicochemical factor that determines the outcome of various biological processes, and nitric oxide (NO) is an essential signalling molecule that controls many cellular processes, including oxidative stress. We previously reported a fluorescent probe that can simultaneously detect intracellular viscosity and NO. As a follow-up study, we intended to investigate the viscosity and nitric oxide of the specific organelles. Herein, we designed and synthesized several probes which can target specific organelle and provide simultaneous fluorescence changes to the viscosity and nitric oxide. Probes can be accumulated in cellular organelles such as mitochondria, lysosomes, endoplasmic reticulum and cytosol. We presented physiological properties of probes in a solution and the living cells. The probes showed distinct fluorescence change in response to elevation of viscosity and NO levels. In addition, we are planning to apply the probes to a disease model regarding the changes in NO and viscosity of specific organelles.

Poster Presentation : **ORGN.P-397**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Development of NAD(P)H-activable fluorescent probes for real-time monitoring in living cells

<u>Yujin Cha</u>, Sun Young Park, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Reduced nicotinamide adenine dinucleotide (NADH) and reduced nicotinamide adenine dinucleotide phosphate (NADPH) are essential coenzymes existed in human cells. NAD(P)H is involved in many biological processes such as energy metabolism, mitochondrial function, biosynthesis, cell death, and aging. In addition, the overexpression of NAD(P)H has been observed in various diseases, including cancer, neoplasia, Parkinson’s and Alzheimer’s diseases. Therefore, NAD(P)H has been considered as a potential target for the diagnosis and the related research fields for drug discovery.In this regard, we developed NAD(P)H-activable fluorescent turn-on probes composed of various intramolecular charge transfer (ICT) acceptor parts possessing different electron withdrawing abilities. In the presence of NAD(P)H, the probes get reduced and exhibit strong ICT emissions with different wavelengths. We expected that the probes can be applied to monitor NAD(P)H in living cells.

Poster Presentation : **ORGN.P-398**

Organic Chemistry

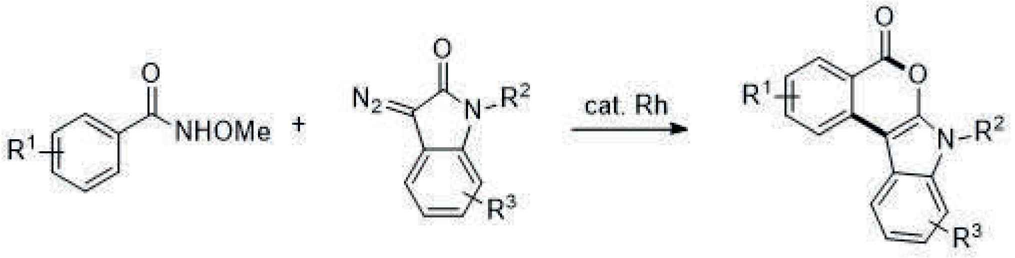
Exhibition Hall 1 FRI 11:00~12:30

Rh(III)-Catalyzed Sequential C–H Activation and Cyclization from *N*-Methoxyarylamides and 3-Diazooxindoles for the Synthesis of Isochromenoindolones

Hee Chan Noh, Gi Hoon Ko, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Since heterocyclic compounds play a very important role in organic synthesis, medicinal chemistry, and materials science, the development of new synthetic methods for these compounds has continued. In the last two decades, tremendous achievements have been made in transition metal-catalyzed C–H functionalization, which has become a convenient method for forming a variety of C–C and C–heteroatom bonds, eventually providing an efficient atom- and step-economical synthetic strategy for heterocyclic compounds without prefunctionalization of the starting material. Indoles represent one of the most important privileged scaffolds and are broadly found in natural products and pharmaceuticals. Driven by its biologically applied potential, the development of an efficient synthetic method for isochromenoindolone is highly required. In a continuation of our studies directed toward the development of novel synthetic methods for heterocycle-fused indole, herein, we have demonstrated sequential Rh(III)-catalyzed C–H activation and cyclization from *N*-methoxyarylamides and 3-diazooxindoles for the synthesis of isochromenoindolones.



Poster Presentation : **ORGN.P-399**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Strategies for ^{18}F Radiolabeling of Covalent Organic Frameworks (COFs) for Multimodality Imaging

Wonhyeok Yun, Ju Gyeong Jeong[1], Kyo Chul Lee[2,*], Dong Wook Kim[*]

Department of Chemistry, Inha University, Korea
[1]*Chemistry, Inha University, Korea*
[2]*Korea Institute of Radiological & Medical Science, Korea*

Covalent Organic Frameworks (COFs), 2D nanomaterials consisting of a single layer of atoms, are increasingly concerned with the recent rapid development of graphene. Due to their crystalline porous structure with facilely tailored functionalities and tunable photophysical properties, COF nanosheets have attracted tremendous attention in biomedical fields. The uniform pore size distribution of COFs may offer more predictable drug release behavior. Moreover, COFs are biocompatible and non-toxic compared to Metal-Organic Frameworks (MOFs) because of the absence of metals. In this work, we introduce synthetic strategies of COFs for pre-targeting Positron Emission Tomography (PET) imaging protocol through the nucleophilic substitution of the mesylate group using a short half-life [^{18}F] Fluoride. For this purpose, mesylate-functionalized PEGylated COF nanosheets were prepared by imine formation between aldehydes and amines. Our goal was to propose a novel method of ^{18}F-labeling of COF nanosheets by optimizing fluorination and applying simple purification with centrifugation. Our study identified a role for COFs as a ^{18}F chelator for PET imaging and also introduced multimodality molecular imaging with combined optical and PET modalities due to the properties of COFs.

Poster Presentation : **ORGN.P-400**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Development of endogenous H_2S-mediated cancer cell-specific gemcitabine activation fluorescent probe and its application

Shin A Yoon, Yujin Cha[1], Min Hee Lee[*]

Department of Chemistry, Sookmyung Women's University, Korea
[1]*Sookmyung Women's University, Korea*

Endogenous H_2S-driven theranostic **H_2S-Gem** have been invented. The theranostic prodrug **H_2S-Gem** is selectively activated in cancer cells, releasing active gemcitabine with a simultaneous fluorescence turn-on. **H_2S-Gem** selectively inhibited cancer cell growth compared to the mother chemotherapeutic gemcitabine. It showed UV-absorption at 400 nm and emission at 505 nm in the presence of exogenous H_2S. Even this theranostic **H_2S-Gem** was activated in the presence of minimal quantity (37 nM) of H_2S. The gemcitabine release process is highly selective toward H_2S, such specific activation allows gemcitabine release exclusively in cancer cells. In vitro cellular images indicated endogenous H_2S level in cancer cells is relatively higher than the normal WI-38 cells. Inhibition assay study indicated that cystathionine β-synthase (CBS) and cystathionine γ-lyase are source of H_2S formation in cancer cells. It showed selective antiproliferative activity exclusive in the cancer cells (HeLa and A549) than the human normal fibroblast cells. Overall, it is a unique protocol for tracking and transporting chemotherapeutic agent to tumor areas without the guidance of tumor-directive ligands.

Poster Presentation : **ORGN.P-401**

Organic Chemistry

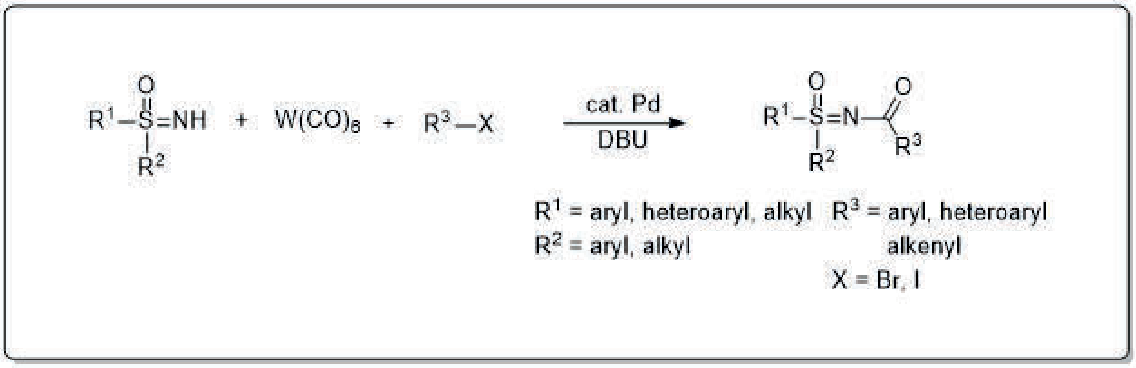
Exhibition Hall 1 FRI 11:00~12:30

Pd(II)-Catalyzed *N*-Carbonylative Cross-Coupling Reaction of Sulfonimines with Aryl, Heteroaryl, and Alkenyl Halides Using Tungsten Hexacarbonyl as Carbon Monoxide Source

Hee Jin Yang, Gi Uk Han, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Sulfoximines have been in the spotlight for decades in medicinal chemistry, agricultural chemistry, and materials science. Sulfoximines are used as building blocks, organocatalysts, directing groups in C−H activation because of their structural variety, hydrogen bonding ability, and high metabolic stability. Therefore, it is necessary to develop a novel synthesis method and functionalization of sulfoximine.We have developed *N*-carbonylation cross-coupling reactions of sulfoximines with a variety of aryl, heteroaryl and aryl halides using a Pd(II)-catalyst and $W(CO)_6$ as a solid source of carbon monoxide. And *N*-acylated sulfoximines was synthesized in good yields. In addition, alkenyl bromide and sulfoximine reacted through palladium(II)-catalyzed *N*-acylation reactions to form *N*-cinnamoyl sulfoximines. This synthetic method has the advantages of a wide substrate range, high functional group tolerance, simple operation, and chemoselectivity between chloride and bromide.



Poster Presentation : **ORGN.P-402**

Organic Chemistry

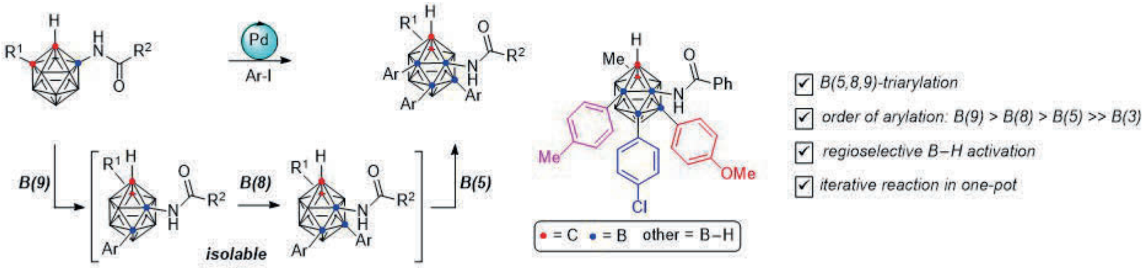
Exhibition Hall 1 FRI 11:00~12:30

Selective B(5,8,9)-Triarylation Reaction of *o*-Carboranes via Determination of the Sequence of Introduction of Aryl Groups into B(4)-Acylamino-*o*-carboranes

Tae Hyeon Kim, Kyungsup Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

The development of a selective synthetic method for polysubstituted carboranes is becoming increasingly important due to the versatile utility of these materials in synthetic, medicinal, and materials chemistry. Although iterative B−H alkylation, arylation, alkenylation, acetoxylation and fluorination have been reported, these reactions are often nonselective and/or uncontrollable. We wondered about the possibility of iterative B−H functionalization in a single operation on a mechanistic platform. Therefore, selective and controllable iterative B−H functionalization based on determination of the order of introduction of substituents into the BH vertices of carborane clusters continues to be a major challenge. Palladium-catalyzed iterative cage B−H arylation reaction of a wide range of B(4)-acylamino-*o*-carboranes with aryl iodides has been developed, leading to the formation of B(5,8,9)-triarylated B(4)-acylamino-*o*-carboranes with excellent regioselectivity. Moreover, B(5,8,9)-triarylated carboranes bearing three different aryl groups were synthesized from B(4)-acylamino-*o*-carborane and three different aryl iodides. The order of introduction [(B(9) > B(8) > B(5)] of aryl groups into the B(5,8,9)-triarylation reaction was determined for the first time through NMR monitoring and X-ray analyses.



☑ B(5,8,9)-triarylation
☑ order of arylation: B(9) > B(8) > B(5) >> B(3)
☑ regioselective B−H activation
☑ iterative reaction in one-pot

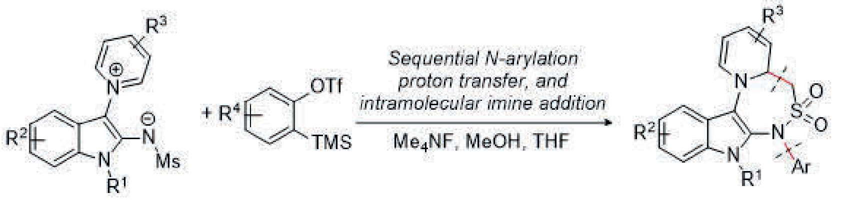
Poster Presentation : **ORGN.P-403**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Sequential *N*-Arylation and Intramolecular Imine Addition Reaction of Arynes with Indoloazomethine Ylides for the Synthesis of Thiadiazepine Derivatives

Tae Hyeon Kim, Kyungsup Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

The 1,4-thiadiazepine skeleton is a privileged structure found in many pharmacologically active compounds. Accompanied by a range of biological activities, the importance of the 1,4-thiadiazepine scaffold in the drug discovery field is well recognized. Because the bioactivity of 1,4-thiadiazepine derivatives has been known to be largely affected through the fusion to various heterocycles, the fusion of this 1,4-thiadiazepine ring with carbo- or heterocycles have been intensively investigated. Thus, a new strategy that is getting a lot of attention lately is to fuse the thiadiazepine moiety with heterocycles for more advanced structure-activity relationship (SAR) investigations. We report the metal-free reaction of indoloazomethine ylides with aryne precursors, leading to the formation of 1,4-thiadiazepines through sequential *N*-arylation, proton transfer, and intramolecular imine addition reaction. Moreover, 1,4-thiadiazepine derivatives were easily converted to produce fully oxidized 1,4-thiadiazepines, which were heated in toluene to furnish indoloindolizines. These transformations can be efficiently accessed in semi one-pot.



☑ *novel scaffold*
☑ *concise one-pot protocol*
☑ *metal—free*
☑ *high selectivity*

Poster Presentation : **ORGN.P-404**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Pinched Tube Flow Reactor with In-Line mixing for Applicable to Mass Production

Yea seul Jang, Chan Pil Park[*]

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

Recently, continuous flow processes have attracted a lot of attention in various fields such as pharmaceuticals and organic synthesis. In particular, the continuous flow system using micro-channels such as glass plates and tubes can be applied industrially as well as in the laboratory. However, when an expensive glass plate is used, there is a problem that it may be clogged due to solid intermediates and products. When the fluoropolymer tube is clogged, it has the advantage of being able to process such as cutting, but a straight tube with a large inner diameter has limited diffusion, so the mixing efficiency of reactants is lowered. In this study, in order to not only solve the above-mentioned problems, but also to increase the mixing efficiency, we are trying to process the tube into various shapes. The pinched tube (processed tube) can efficiently and economically build a continuous flow system, so they can be applied in industrial fields that require mass production.

Poster Presentation : **ORGN.P-405**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

gem-Dichlorocyclopropane Synthesis using Inorganic Salt Powder

Seula Yun, Chan Pil Park*

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

gem-Dichlorocyclopropane is considered important in pharmaceutical and biological applications because of their high reactivity and availability. Conventionally, the reaction was carried out through liquid-liquid biphasic system using water and an organic solvent. However, due to limitations such as mass transfer, there are problems in that the reaction proceeds slowly or the side reaction is accelerated. In this study, to solve the problem of liquid-liquid biphasic system, dichlorocarbene was formed by applying a solid-liquid system with powder inorganic salt and liquid chloroform. The formed dichlorocarbene was reacted with styrene to synthesize *gem*-dichlorocyclopropane. The method may proceed the reaction more effectively by using a solid-liquid system and is more economical and environmentally than conventional method.

Poster Presentation : **ORGN.P-406**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

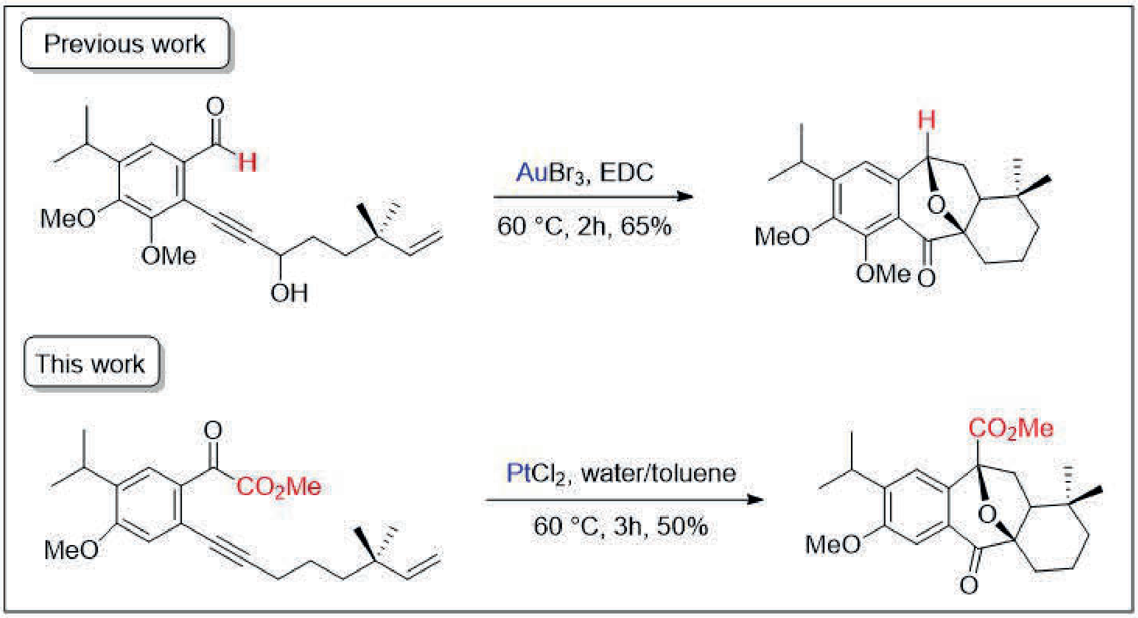
Metal-transition catalyzed cyclization reaction leading to oxacyclic ring systems with ester functional group

Juhui Lee, Le Thuy Quynh[1], Chang Ho Oh*

Department of Chemistry, Hanyang University, Korea

[1]*Chemistry department, Hanyang University, Korea*

The benzannulated oxygen-bridged seven-membered ring systems have been found in various biologically active compounds (brussonol, salviasperano, przewalskin E…). We report herein a convenient method for the preparation of these oxacyclic ring systems with ester functional group via metal-transition catalyzed cyclization reaction, which could bring useful intermediates in the synthesis of natural products.



Poster Presentation : **ORGN.P-407**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

[Withdrawal] Cobalt-Catalyzed Intermolecular C(sp^3)–H Amidation of Unactivated Hydrocarbons

Jeonghyo Lee, Seongho Jin[1], Dongwook Kim[2], Soon Hyeok Hong[1,*], Sukbok Chang[1,*]

Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, Korea
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*
[2]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

- Withdrawal -

Poster Presentation : **ORGN.P-408**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Generation and functionalization of α-anionic tetrahydropyran in flow

Dongyong Kim, Hyune-Jea Lee, Heejin Kim*

Department of Chemistry, Korea University, Korea

Tetrahydropyran (THP) ring is a common structural motif in bioactive natural compounds including therapeutic agents. However, the direct method for α-C-H functionalization of THP is rare and remains a challenging issue because of the rapid and uncontrollable decomposition of anionic cyclic ethers. Herein we report that the generation of α-anionic THP and its serial reaction with various electrophiles is accomplished in flow. The unstable α-anionic THP intermediate was effectively generated to react with various electrophiles using a flow microreactor with precise control of residence time and reaction condition. Also, the continuous-flow reaction manner enabled the gram-scale synthesis of α-borylated THP in high productivity, which is available in cross-coupling reaction.

Poster Presentation : **ORGN.P-409**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Electrochemical Oxidation of 5-Hydroxymethylfurfural (HMF)

Kookhee Kang, Jong Min Park, Chan Pil Park*

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

5-Hydroxymethylfurfural (HMF), obtained through biomass conversion, can be converted into useful substances such as 2, 5-diformylfuran (DFF), 2, 5-furandicarboxylic acid (FDCA) and so on. DFF is used as a versatile bio-based platform chemical used as a multi-purpose chemical intermediate, and FDCA is used as a substitute for terephthalic acid used in polyester manufacturing or as a raw material for succinic acid production. In the general oxidation process of HMF, an excessive amount of catalyst was used or the reaction was carried out under harsh conditions. In this study, oxidation of HMF was performed under milder conditions than conventional reactions by applying an electrochemical system. In addition, it could suggest that more green and economical methods can be proposed.

Poster Presentation : **ORGN.P-410**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis of various benzofuran-2,3-diones and its derivatives

Seunghwan Ham, **Chang Ho Oh***

Department of Chemistry, Hanyang University, Korea

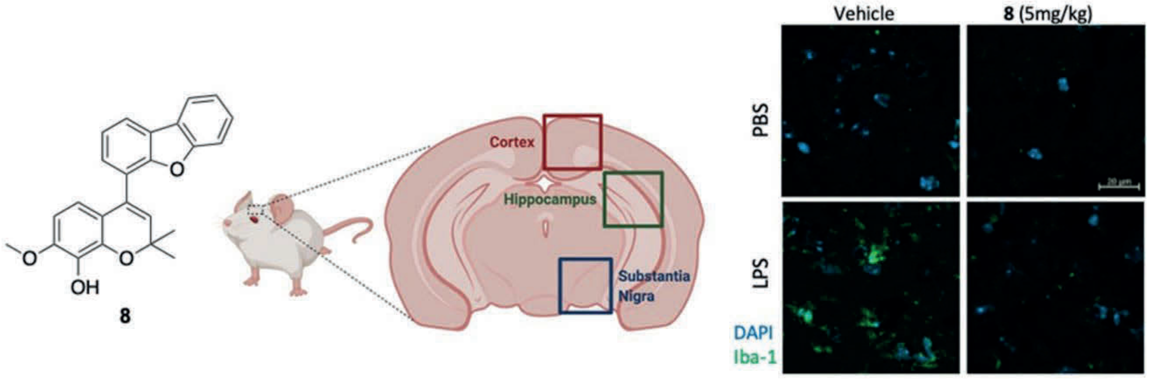
Poster Presentation : **ORGN.P-411**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Phenotype-based Screening Discovered a Benzopyran-embedded Microtubule Inhibitor as an Anti-neuroinflammatory Agent

Jaeseok Lee, Jongmin Park*, Seung Bum Park[1,*]

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

Neuroinflammation has been reported as one of the major process resulting central nerve system (CNS) diseases. Therefore, alleviation of the neuroinflammation has been spotlighted for the treatment of CNS diseases. Herein, we discovered benzopyran-embedded tubulin inhibitor 1 as an anti-neuroinflammatory agent from phenotype-based screening. Photoaffinity based target protein binding site study showed that compound 1 bound to the colchicine-binding site of tubulin. Following structure-activity relationship (SAR) study generated compound 8 as a lead compound with enhanced efficacy for anti-neuroinflammation. Compound 8 regulated two major inflammatory pathways, NF-kB pathway and NLRP3 inflammasome formation. The mode-of-action study revealed that upregulation of tubulin monomer was the key factor for anti-neuroinflammatory activity of compound 8. We unexpectedly found that the upregulated tubulin monomer recruited p65, inhibited its translocation from cytosol to nucleus, and blocked NF-kB mediated inflammatory pathways. We further validated compound 8 induced amelioration of microglia activation by downregulation of lba-1 and cytokines in neuroinflammatory mouse model. Our study suggests microtubule regulation as a potential anti-neuroinflammatory therapeutic strategy for CNS disease treatments.


O
O
OH
8
Cortex
Hippocampus
Substantia Nigra
Vehicle
8 (5mg/kg)
PBS
LPS
DAPI
Iba-1
20 μm

Poster Presentation : **ORGN.P-412**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Continuous Flow Reaction Based on Silica Gel and Magnetic Bead Catalyst

<u>Jong Min Park</u>, Yea Seul Jang, Chan Pil Park[*]

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

Silica gel is used as an efficient support for catalysts due to its high chemical and thermal stability and high surface area to volume. Also, the silica coated magnetic bead has magnetism, so it can be easily separated. The continuous flow system has advantages such as high surface area to volume ratio, short diffusion distance and high mixing efficiency, and can achieve high catalyst activity due to the wide interface between solid catalyst and liquid phase. However, when solids such as silica gel are used in a continuous flow system, they may aggregate with each other or precipitate in the reactor, which may prevent the stable flow of the fluid. To solve this problem, we measured the dispersion stability of silica gel and solvent, injected silica gel stably in a suspension method, and injected immiscible liquid phase to create a liquid-liquid slug flow. Chemical reactions such as transesterification, hydrogenation, and Suzuki-Miyaura reaction were used to confirm that this method stably provided the catalyst to each slug.

Poster Presentation : **ORGN.P-413**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Ir(NHC) catalyzed Intermolecular Cross-Coupling and intramolecular cyclization of alcohols

Mi-hyun Lee, Heemin Byeon[1], Hye-Young Jang[2,*]

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

Transition metal-catalyzed borrowing hydrogen strategy in C-C bond formation of alcohols provides environmental advantages over traditional approaches where stoichiometric amounts of inorganic halide byproducts are formed. For such conversion, transition metal catalysts having NHC ligands have been actively studied due to their interesting chemical properties.The Ir(NHC) catalyst possessing triscarbene ligands is effective in synthesizing α-alkylation of ketone and β-alkylation of secondary alcohol through intermolecular coupling and intramolecular cyclization of diols.In this study, a variety of substrates for such conversions along with the mechanism will be presented.

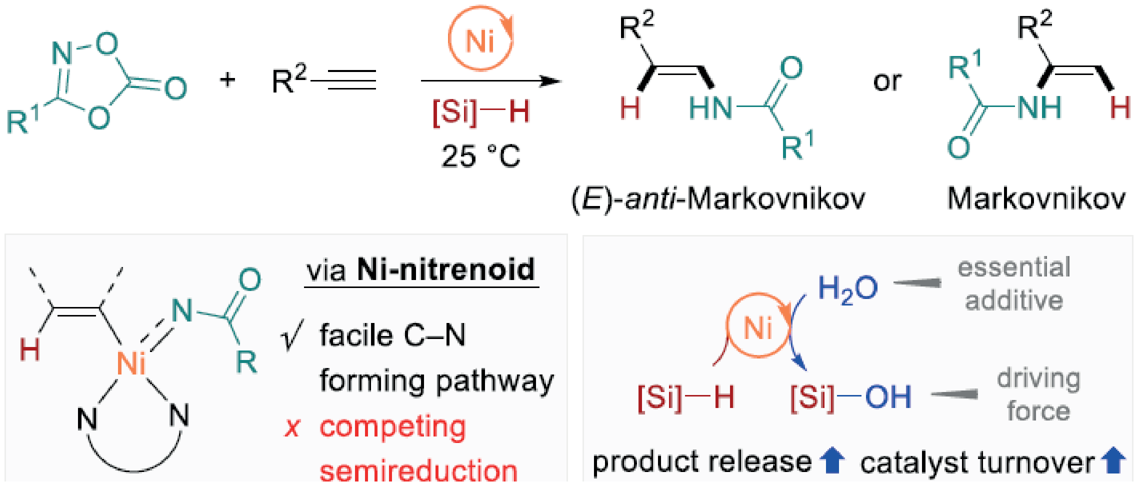
Poster Presentation : **ORGN.P-414**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Merging NiH Catalysis and Inner-Sphere Metal-Nitrenoid Transfer for Hydroamidation of Alkynes

Xiang Lyu, Sukbok Chang[1,*]

Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, Korea
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

The formal hydroamination/hydroamidation utilizing metal hydride is an appealing synthetic tool for the construction of valuable nitrogen-containing compounds from unsaturated hydrocarbons. While significant advances have been made for the functionalizations of alkenes in this realm, the direct hydroamidation of alkynes remains rather limited due to the high feasibility of the key metal-alkenyl intermediate to choose other reaction pathways. Herein, we report a NiH-catalyzed strategy for the hydroamidation of alkynes with dioxazolones, which allows convenient access to synthetically useful secondary enamides in (*E*)-*anti*-Markovnikov or Markovnikov selectivity. The reaction is viable for both terminal and internal alkynes and is also tolerant with a range of subtle functional groups. With H_2O found as an essential component for high catalyst turnovers, the involvement of *inner-sphere* nitrenoid transfer is proposed that outcompetes an undesired semireduction process, thus representing the first example to show the competence of Ni catalysis for metal-nitrenoid formation from dioxazolones.


N–O
O
O
R1
+
R2
Ni
[Si]—H
25 °C
R2
H
HN
O
R1
or
R2
R1
O
NH
H
(E)-anti-Markovnikov
Markovnikov
H
Ni
N
O
R
N
N
via Ni-nitrenoid
√ facile C–N forming pathway
x competing semireduction
H2O
essential additive
Ni
[Si]—H
[Si]—OH
driving force
product release
catalyst turnover

Poster Presentation : **ORGN.P-415**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthetic optimization for N-nitration reaction of Pyrazole

Kuktae Kwon*, Hae-Wook Yoo, So Jung Lee, SeungHee Kim

Agency for Defense Development, Korea

2,4,6-Trinitrotoluene(TNT) is still using as a melt-cast explosive from 1890s. There had been many attempts to replace TNT for improving performance. Several candidates were derived, but critical defects were found during development processes such as scale-up, melting and so on.Recently, 3,4-Dinitropyrazole(DNP) had been reported as a promising candidate for replacement of TNT. The first step for synthesis of DNP is N-nitration reaction of pyrazole to 1-Nitropyrazole, and this is extremely exothermic reaction. Moreover, stirring was not enough because large amount of precipitate was formed during the nitration reaction. This could cause partial heat accumulation, and it can be dangerous for large scale synthesis. So our group researched about control of reaction heat and precipitation for this reaction.

Poster Presentation : **ORGN.P-416**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Characterization of Stable Ni(II) Radical Cation of Diazatriphenylene Embedded Corrole Analogue

Chang Hee Lee[*], **Srinivas Samala**[1]

Department of Chemistry & Biochemistry, Kangwon National University, Korea
[1]*Chemistry, Kangwon National University, Korea*

The chemistry of π-extended corroles are hampered due to the synthetic challenges due to the limited availability of proper synthetic precursors. Incorporation of bipyridine unit as a part of the corrinoid macrocycles are more challenging. Apart from the traditional tri anionic corroles, bipyridine-incorporated corroles act as monoanionic ligand, and thus can stabilize low oxidation state of coordinated metal ions. The system can display a unique electronic, structural and spectroscopic properties. With these regards, A π-extended, diaza-triphenylene embedded corrole analogue and its Ni(II)-complex was synthesized from diaza-triphenylene diketone precursor. The synthesis accomplished by series of reactions involves reduction of diketone to diol followed by condensation with pyrrole to afford dipyrromethane intermediate. Acid-catalyzed condensation with pentafluorobenzaldehyde afforded the mono-anionic π-extended corrole analogue containing two pyridine moieties. The free base acts as a redox non innocent ligand. Metal insertion is accomplished by reaction with Ni(OAc)2.4H2O and unexpectedly, the reaction resulted in the formation of air stable Ni(II)-cation radical, which can be converted to Ni(II) cation upon treatment with single electron oxidant.

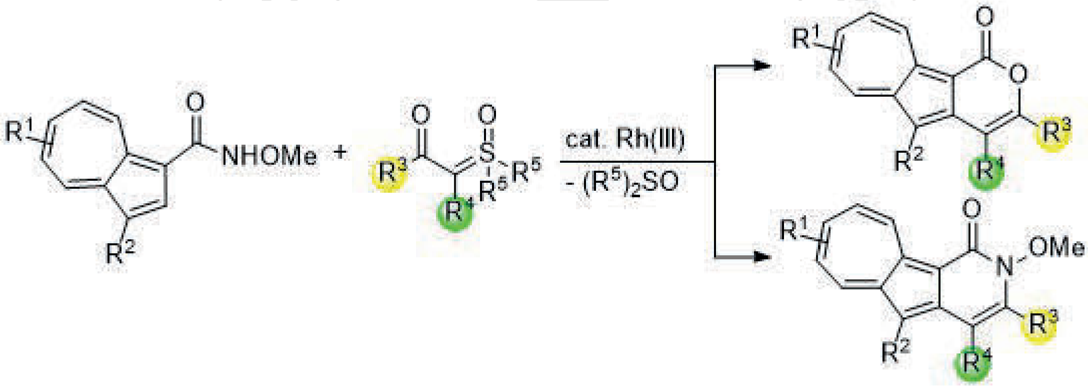
Poster Presentation : **ORGN.P-417**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Regioselective and Chemodivergent Synthesis of Azulenolactones and Azulenolactams from Rh-Catalyzed Reactions of Azulenecarboxamides with Sulfoxonium Ylides

Hanjoong Kim, Hee Chan Noh, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

A regioselective and chemodivergent synthetic approach for azulenolactones and azulenolactams as a new scaffold was demonstrated through Rh(III)-catalyzed reaction of *N*-methoxyazulene-1-carboxamides with sulfoxonium ylides. Sulfoxonium ylides that act as a precursor of secondary carbene was described, leading to the selective formation of azulenolactones and azulenolactams bearing two substituents on a newly introduced double bond. This method demonstrated functionalization of less reactive 2-position of azulene to overcome the natural reactivity.



Poster Presentation : **ORGN.P-418**

Organic Chemistry

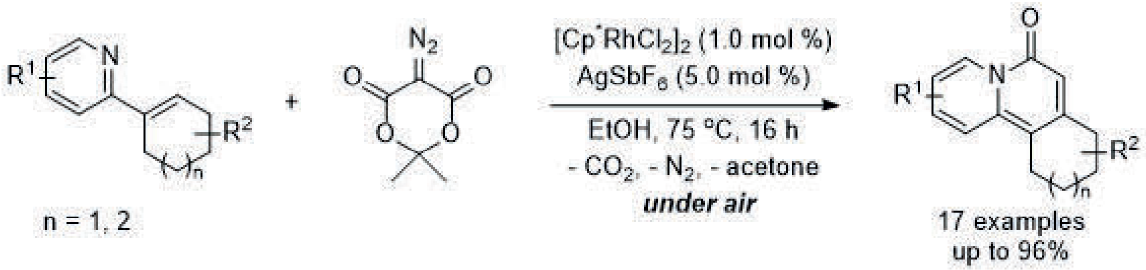
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Quinolizinones from Rh-Catalyzed C–H Activation Reaction of 2-(1-Cycloalkenyl)pyridines with Diazo Meldrum's Acids

Hanjoong Kim, Kyungsup Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

The development of new synthetic methods for the nitrogen-containing heterocyclic compounds is very important in the research area related to new medicines, drug discovery, fine chemicals, and active pharmaceutical ingredients (API). In particular, quinolizin-4-one is one of the important azaheterocyclic scaffolds found primarily in the core structure of molecules with biological activity. Recently, we developed the synthetic approach for quinolizin-4-one derivatives through sequential diazotization, Co(0)-catalyzed carbonylation, and intramolecular cyclization reaction under carbon monoxide atmosphere. Stimulated by these results, we envisioned that if 2-(1-cycloalkenyl)pyridines were treated with transition metal catalyst in the presence of diazo Meldrum's acid, a variety of cycloalkyl-fused quinolizin-4-one derivatives would be produced through C–H activation reaction together with the release of carbon dioxide, molecular nitrogen gas, and acetone. Herein, we report a new synthetic method for quinolizin-4-ones from the reaction of 2-(1-cycloalkenyl)pyridine derivatives with diazo Meldrum's acids through C–H activation reaction.



- Novel quinolizin-4-ones
- Low loading Rh-catalyst
- Fluorescent materials

$\lambda_{max,\ abs}$ (nm) : 391 to 393

$\lambda_{max,\ em}$ (nm) : 472 to 493

ϕ (%) : 7% - 24%

Poster Presentation : **ORGN.P-419**

Organic Chemistry

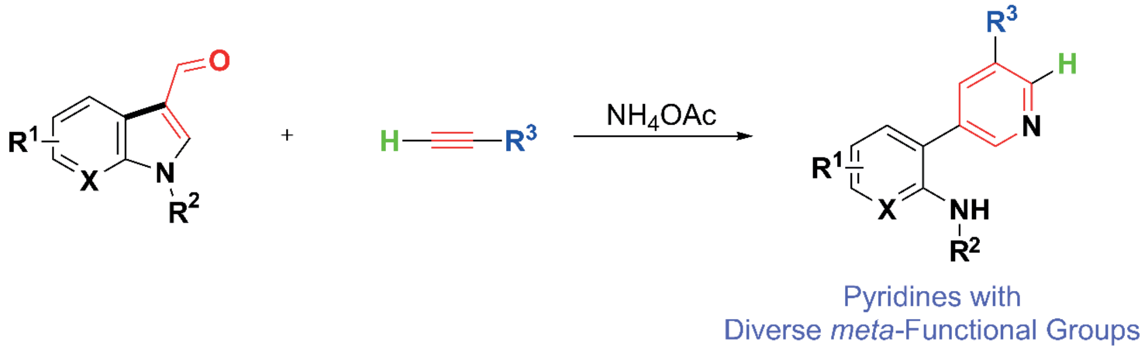
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of diversely meta-substituted 3-(2aminoaryl)pyridine via remodelling of (aza)indoles

Sihyeong Yi, Seung Bum Park*

Division of Chemistry, Seoul National University, Korea

meta-Substituted pyridines are widely found among natural products and drug molecules. One of the most symbolic example is niacine, or vitamine B3, which is one of the essential nutrients to our body. Despite the importance of meta-substitued pyridines as structural motif in drugs, synthetic methods for diverse meta-substitued pyridines are highly limited. One of the most traditional and general method is Bohlmann-Rhatz synthesis, but this method generates inevitable ortho-substitution. To solve this problem, we envisioned the remodelling of 3-formyl (aza)indoles with in situ generated beta-amino acrylates. With this method, we generated diverse 3-(2aminoaryl)pyridines with diverse meta-substituents including ester, sufone, phosphonate, amide-analogous aryls, and etc. Also we succeeded late-stage conjugation between actual drug molecules and core-remodelling of natural products and drug molecules. We expect this synthetic methodology reach yet touched chemical space.



Poster Presentation : **ORGN.P-420**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Ionic Liquid Functionalized Calix Arene as a Phase Transfer Catalyst for Nucleophilic Fluorination

Minji Nam, Su Jin Park, Geunhyuck Bak, Dong Wook Kim*

Department of Chemistry, Inha University, Korea

Nowadays, there has been significant growth in interest in the synthesis of fluorine-containing organic molecules through nucleophilic substitution reactions. Hence, new types of calix arene based organic catalysts are synthesized, which are tethered with imidazolium based ionic liquid. These can be served as highly efficient catalysts for nucleophilic substitution reactions using alkali metal fluoride, especially potassium fluoride. In this study, catalytic activity has been investigated by comparing widely used catalysts and optimizing reaction conditions. Various substrates, more than 10 chemical compounds, are tested with newly produced catalyst under optimized reaction conditions and most of them show good reactivity and selectivity. Therefore, catalyzed nucleophilic fluorination method illustrates extremely high performance in base-sensitive substrates, as well as various types of substrates.

Poster Presentation : **ORGN.P-421**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Lysosome localised lipid and protein oxidation to perturb autophagy after dysfunction of lysosome and its fusion

Mingyu Park, Jung Seung Nam, Taehyun Kim[1], Duyoung Min, Taiho Park[1], Tae-Hyuk Kwon*

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

Lysosome target iridium complexes produce reactive oxygen species and damage lysosomal proteins and membrane. In this project, we provide chemical description on how sophisticated ROS generation disturbs autophagic flux. In-depth proteomic analyses were conducted to verify proteins of which methionine, arginene, or lysine residues are significantly oxidized. Further investigations on cell death phenotype show a plausible link between photosensitization of the iridium complexes and autophagy perturbation after lysosomal dysfunction.

Poster Presentation : **ORGN.P-422**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Relief of Excited-State Antiaromaticity Enables Single-Benzene White Emitters

Younghun Kim, Heechan Kim, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Aromatic benzene becomes antiaromatic upon photoexcitation, and takes various relaxation pathways to alleviate the antiaromaticity. Single-benzene fluorophores (SBFs) are benzene-based molecules that exploit this excited-state process for light emission at visible energy window. We present new SBFs having acidic N–H protons and adjacent acetyl groups, which trigger intramolecular proton transfer (ESIPT) upon photoexcitation. Remarkably, these molecules exhibit dual emissions from the locally excited (LE) state and the ESIPT state, which compete and complement with each other to produce white light in both solution and solid-state. Our theoretical analysis suggests that structural relaxation to strengthen two pairs of intramolecular hydrogen bonds, in conjunction with the complete transfer of a single proton, is responsible for the relief of excited-state antiaromaticity. These molecules represent the first example of SBFs harnessing two different photophysical pathways to generate white light from a small benzene core. This presentation will discuss a new design strategy for developing single-molecule dual-emitters and their technological applications in white light-emitting devices.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

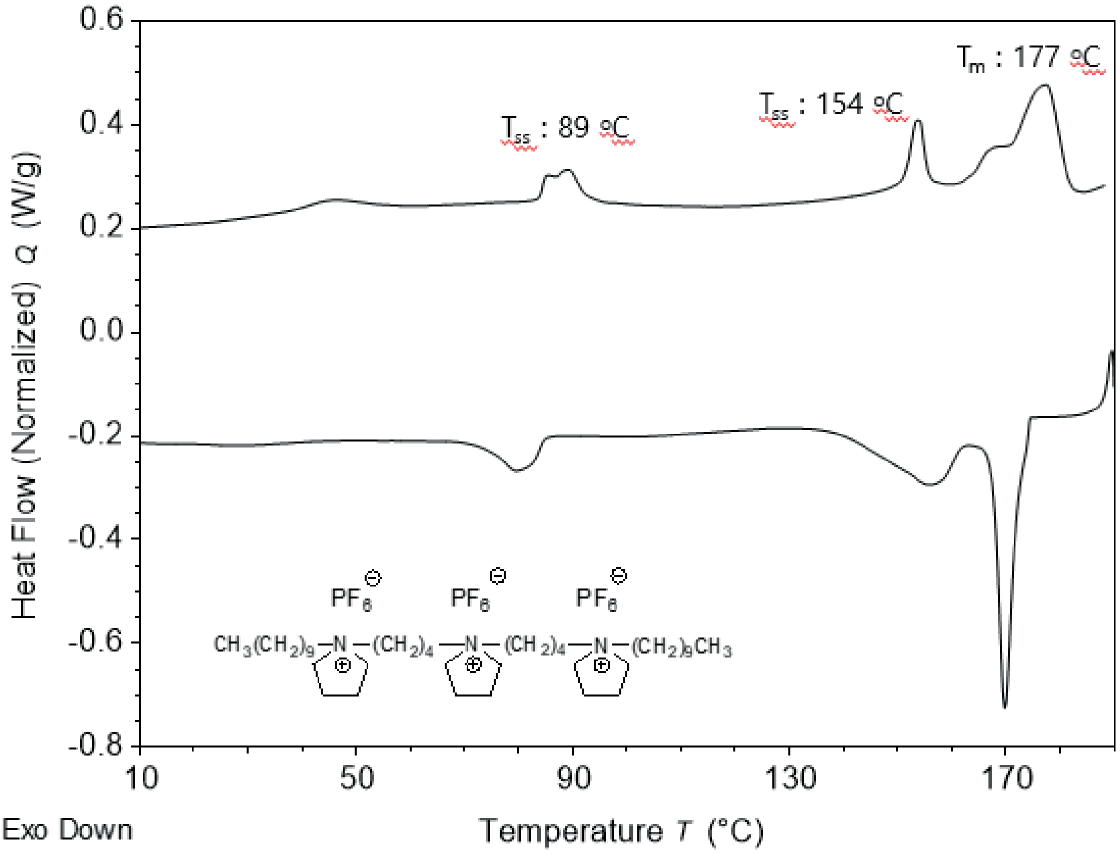
Poster Presentation : **ORGN.P-423**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Tricationic Pyrrolidinium Salts and Their Thermal Properties

Jongchan Shin, Minjae Lee*

Department of Chemistry, Kunsan National University, Korea

In the solid-state electrolyte system, ion density and ion dissociation are important factors to enhance the target ion transfer behaviors. In our research group, various structures of ammonium-based organic dications have been reported. In this presentation, a series of pyrrolidinium-based tricatons are synthesized and characterized. The most C_4 alkylene bridged tris-pyrrolidinium Br^-, BF_4^-, PF_6^- salts show solid-solid phase transitions and corresponding Tf_2N^- salts are room temperature ionic liquids(RTILs). Thermal gravimetric analysis show their thermal stabilities; halide salts are less stable than BF_4^-, PF_6^- or Tf_2N^- salts. The trication with n-decyl alkyl substituent with PF_6^- show a relatively small entropy of fusion, $\Delta S_f = 27$ J mol^{-1} K^{-1}, which is a close value to the Timmermans' definition of plastic crystals ($\Delta S_f < 20$ J mol^{-1} K^{-1}).


0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
Heat Flow (Normalized) Q (W/g)
10
50
90
130
170
Temperature T (°C)
Exo Down
T_ss : 89 ºC
T_ss : 154 ºC
T_m : 177 ºC
PF6
PF6
PF6
CH3(CH2)9
(CH2)4
(CH2)4
(CH2)9CH3
N

Poster Presentation : **ORGN.P-424**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Cu(NHC)-catalyzed cyclization of propargyl amines and CO2

Seong Eon Kim, **Hye-Young Jang**[1,*]

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

Due to increased carbon dioxide emissions, utilization of CO2 forming useful chemicals has been conducted with an expectation to reduce the concentration of CO2 in the air. Synthesis of 2-oxazolidinone from CO2 via transition metal-catalyzed cyclization is one of CO2 utilization techniques. Most previous studies require large excess bases or high pressure of carbon dioxide. Triscarbene-modified Cu(NHC) catalysts are employed in this cyclization under 1 bar of CO2 and base-free conditions. Detailed optimization conditions and the substrate scope are presented.

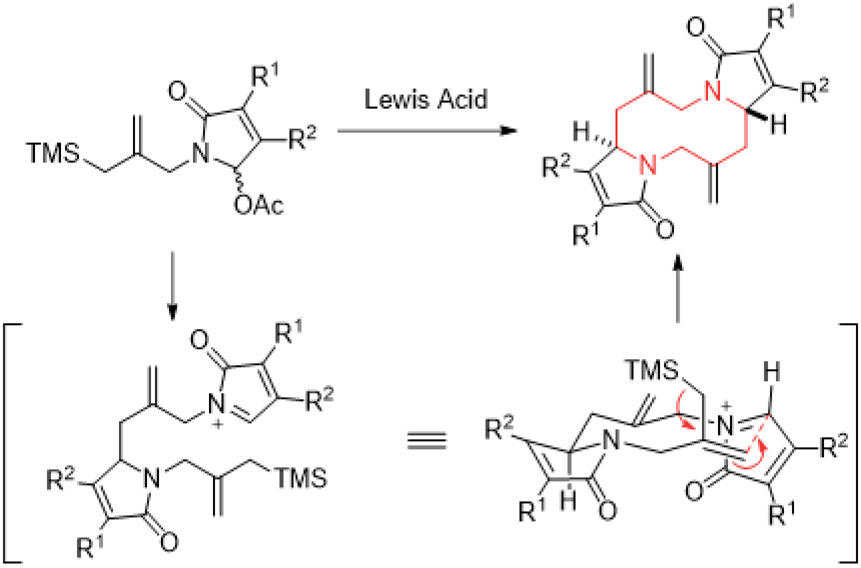
Poster Presentation : **ORGN.P-425**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Intermolecular double aza-Prins cyclization: stereoselective synthesis of 1,6-diazecanes

Gyeongun Kim, Jaekyun Lee[1], Hwasun Yang[2], Sun-Joon Min[3,*], Taek Kang[4,*], Yong Seo Cho[4,*]

Department of Chemistry, Kyung Hee University, Korea
[1]*Chemoinformatics Research, Korea Institute of Science and Technology, Korea*
[2]*Department of Chemistry, Korea University, Korea*
[3]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*
[4]*Korea Institute of Science and Technology, Korea*

Medium-sized heterocycles are commonly founded in various natural products and pharmaceutical active compounds. In spite of its importance, owing to both enthalpic and entropic barriers by ring strain, it remains still a major synthetic challenge to develop the practical and facile methods. Previously, we reported the stereoselective synthesis of 1,6-dioxecane from allenyl silane and aldehyde through an intermolecular double Prins-type cyclization. On the basis of prior study, herein we described the stereoselective synthesis of 1,6-diazecanes. An *N*-acyliminium ion intermediate was generated by dimerization and subsequent intramolecular cyclization was occurred to provide desired 1,6-diazecanes. Our double aza-Prins strategy provided a very concise method for the synthesis of complex azacycles.


TMS
N
O
R1
R2
OAc
Lewis Acid
H
N
O
R1
R2
N
O
R1
R2
H
N+
TMS
≡
TMS
H
N+
R2
R1
O
N
R2
R1
H
O

Poster Presentation : **ORGN.P-426**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

π-bridge effect by adjusting the location and number of thiophenes.

Jinhan Lee, Won Ki Lee[1], Youngeup Jin*

Engineering Chemistry, Pukyong National University, Korea
[1]*Polymer Engineering, Pukyong National University, Korea*

The world energy demand and consumption are growing phenomenally fast all over the world. However, fossil fuels such as coal, natural gas and oil are limited in use. To solve this problem, a majority of advanced countries and scientists have put their efforts on innovating and developing novel and renewable energies. Various eco-energies are being studied, and solar cells have long been studied as endless energy sources that do not generate additional environmental pollution byproducts. Organic solar cells, which have been studied a lot, can be produced at a low price and are easy to mass-produce because they can be worked in a liquid state. In OPVs, donor was synthesized into the alternating structure of push unit and full unit by studying the photoactive layer of organic solar cells, and systematically studied the effect on organic solar cells by controlling the location and number of thiophene widely used as π-bridge. In this study, three type of polymers were synthesised. one is PBDT-mFPz, other is PBDT-T-mFPz, the other PBDT-DT-mFPz. Here, HOMO decreased as thiophene bridge increased. As a result, PBDT-DT-mFPz showed the best performance that 5.117mA/ cm2 of Jsc, 0.592V of Voc and 1.664 of PCE.

Poster Presentation : **ORGN.P-427**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Straightfoward Synthesis of 2-Azetidinyl Pyridine Using Borane as a Protecting Group for Pyridine

Hwasun Yang, **Taek Kang**[1,*]

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

Azetidines are appealing synthetic targets for occurrence in diverse biologically active molecules. A considerable number of synthetic routes toward azetidine moiety have been developed, involving double alkylation of primary amine with 1,3-diactivated propane moiety. However, the alkylation strategy cannot be applied to the synthesis for 2-azetidinyl pyridines from 2-aminopyridines due to nucleophilicity of pyridine which leads to unwanted 6-membered ring formation. For this reason, 2-azetidinyl pyridine has been generally synthesized by S_NAr reaction with 2-halopyridines or other multi-step reactions under harsh conditions. Reported herein is a mild, one-pot synthetic method for 2-azetidinyl pyridines from readily available 2-aminopyridines using borane as a protecting group for nucleophilic nitrogen of pyridine.

Poster Presentation : **ORGN.P-428**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mechanochemical Fluorination of Unactivated C(sp^3)–H Bond

Sehye Min, Soon Hyeok Hong*

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

Mechanochemical organic synthesis furnishes an environmentally benign alternative to traditional organic synthesis by eliminating the use of bulk solvents. The solvent-free or solvent-less reaction conditions could allow close contact between reactants, reducing reaction times. Mechanochemical C–H bond functionalization further offers an atom-economical synthetic method. Although various mechanochemical C(sp^2)–H bond functionalizations have been developed, C(sp^3)–H functionalization is still limited to α-C(sp^3)–H bonds of 1,3-dicarbonyl compounds and ketones.[1] Only recently, the mechanochemical functionalization of unactivated alkanes was uncovered; the Schüth group reported chlorination of methane using trichloroisocyanuric acid (TCCA),[2] and the Zhong group reported Rh(II)-catalyzed C–H amination.[3] Here, we present direct, mechanochemical fluorination of unactivated C(sp^3)–H bonds using N-fluorobenzenesulfonimide (NFSI) as a fluorine source. The observed primary kinetic isotope effect (k_H/k_D = 4.9) is consistent with irreversible hydrogen atom abstraction. The reaction mechanism is currently under investigation.References1. Zhao, S.; Li, Y.; Liu, C.; Zhao, Y. Tetrahedron Lett. 2018, 59, 317.2. Bilke, M.; Losch, P.; Vozniuk, O.; Bodach, A.; Schüth, F. J. Am. Chem. Soc. 2019, 141, 11212.3. Lu, X.; Bai, Y.; Qin, J.; Wang, N.; Wu, Y.; Zhong, F. ACS Sustainable Chem. Eng. 2021, 9, 1684.

Poster Presentation : **ORGN.P-429**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Deep HOMO using Cyano group instead of Fluoro group in OSCs.

Jinhan Lee, Won Ki Lee[1], Youngeup Jin*

Engineering Chemistry, Pukyong National University, Korea
[1]*Department of Polymer?Engineering, Pukyong National University, Korea*

Active research is underway as solar cells have begun to attract attention as alternative energy sources. Various studies are being conducted to increase the efficiency of organic solar cells. A pull type unit may have a lower HOMO when synthesized into a polymer chain by introducing an electron withdrawing group. In this study, novel polymers were synthesized using cyano groups instead of fluorine groups used in previous experiments. In this experiment, PBDT-dCNPz is expected to exhibit a lower HOMO than PBDT-dFHPz. Through this experiment, we wanted to make a high Voc with low HOMO. The polymers,(PBDT-dCNPz, PBDT-dFHPz) were synthesized by stille coupling reaction, and all polymer dissolved in CF and CB at high temperature. The thermal stability of the polymers was measured by Thermo gravimetric analysis (TGA), and at 5% weight loss, the polymers showed over 330℃. PBDT-dFPz and PBDT-dCNPz showed maximum absorption spectra at 508 nm and 580 nm, respectively, with maximum peaks at 711 nm and 802 nm in the film state. The HOMO values for each substance measured by CV were -5.25eV for PBDT-dFPz and -5.51eV for PBDT-dCNPz, which showed that PCE for PBDT-dCNPz was 2.02% lower than PBDT-dFHPz, which was 4.14%. However, the withdrawing group of PBDT-dCNPz is strong and the HOMO value is deeper at 0.26 eV, indicating the possibility that PBDT-dCNPz will be used as a acceptor rather than a donor.

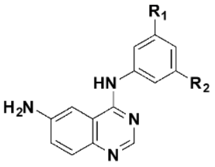
Poster Presentation : **ORGN.P-430**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

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

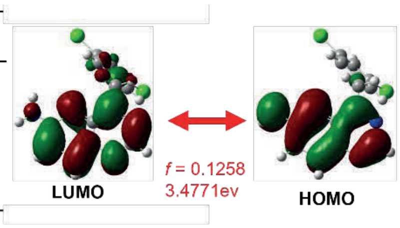
Woojeong Lim, **Eunha Kim**[1,*], **Jongmin Park**[2,*]

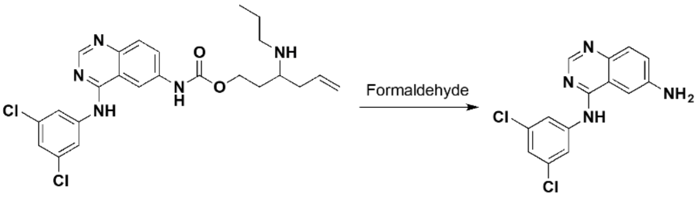
Department of Chemistry, Kangwon National University, Korea
[1]*Department of Molecular Science and Technology, Ajou University, Korea*
[2]*department of Chemistry, Kangwon National University, Korea*

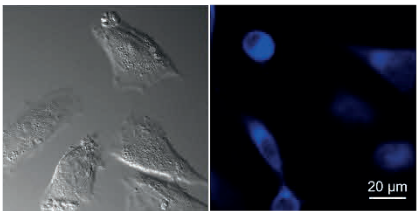
We serendipitously discovered N^4-Phenyl quinazoline-4,6-diamine as a fluorescent scaffold with turn-on characteristics. To improve the photophysical property of the initial fluorescence molecule, we synthesized the derivative of the N^4-Phenyl quinazoline-4,6-diamine. Among those compounds, we observed enhanced fluorescence intensity of the molecule when the phenyl moiety was substituted with electron withdrawing group. By considering quantum yield and cellular uptake, we choose N^4-dichlorophenyl quinazoline-4,6-diamine as a potential fluorophore for various biological applications. As a proof of concept, we developed formaldehyde (FA) fluorescent probe by tailoring amine on 6-position of N^4-dichlorophenyl quinazoline-4,6-diamine. The probe could detect FA via 2-aza-Cope rearrangement. The probe showed the detection limit of 100 nM FA and excellent FA selectivity. Finally, FA could be detected with the probe in the HeLa cells.



#	R^1	R^2	E$_h$^{a}	λ$_{abs}$^{b}	λ$_{Ex}$^{c}	λ$_{Em}$^{d}	Φ$_F$ (%)^e
1	H	H	-0.243	354	365	477	5.9
7a	OMe	OMe	-0.209	359	363	458	2.0
7b	Me	H	-0.238	357	365	467	1.5
7c	CN	H	-0.265	359	363	470	53.5
7d	F	F	-0.250	358	364	474	0.0
7e	Br	Br	-0.249	369	365	467	57.5
7f	Cl	Cl	-0.255	360	366	478	60.9







Poster Presentation : **ORGN.P-431**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Stereoselective Dehydroxylative Cross Coupling via α–Aziridinyl Intermediates.

Hyun-Joon Ha*, Jala Ranjith[1]

Department of Chemistry, Hankuk University of Foreign Studies, Korea
[1]*Department of chemistry, Hankuk University of Foreign Studies, India*

A Lewis acid-mediated stereoselective dehydroxylative cross coupling of aziridyl benzyl alcohols and electron-rich arenes or 2-naphthol was demonstrated. N-substituted α–methyl benzyl group of aziridine substrates was a highly efficient chiral directing group to provide α,α-diaryl aziridines with excellent stereoselectivity. Olefinic intermediates were proposed as a crucial intermediate, and DFT computation indicated the stereoselectivity is originated from the thermodynamic control for the formation of the intermediates.

Poster Presentation : **ORGN.P-432**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Outpacing Intramolecular Rearrangement through Enhanced Mixing in High-Resolution 3D-Printed Metal Flow Microreactor

Hyune-Jea Lee, Heejin Kim, Dong Pyo Kim[1,*]

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

High-resolution 3D-printed stainless steel metal microreactors (3D-PMRs) with different cross-section were manufactured to control ultrafast intramolecular rearrangement reactions in a comparative manner. The 3D-PMR-C (cross section: circular channel) demonstrated the improved controllability in rapid Fries-type rearrangement reactions, because of the superior mixing efficiency compared with rectangular cross-section channels (250 μm x 125 μm) which was confirmed based on the computational flow dynamics (CFD) simulation. Even in case of very rapid intramolecular rearrangement of sterically small acetyl group occurred in 333 μs of reaction time, the desired intermolecular reaction could outpace to the undesired intramolecular rearrangement using 3D-PMR to result in high conversion and yield.

Poster Presentation : **ORGN.P-433**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Highly Efficient and Robust Iron Catalytic System for Intramolecular C(sp$_3$)–HAmidation Leading to γ-Lactams

Jeonguk Kweon, Sukbok Chang*

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

We herein disclose the use of an iron catalyst system for an intramolecular C–H amidation toward γ-lactam synthesis from dioxazolone precursors. (Phthalocyanine)Fe(III)Cl was found to catalyze this cyclization with extremely high turnover numbers up to 47,000 under mild and aerobic conditions. On the basis of experimental and computational mechanistic studies, the reaction was suggested to proceed via a stepwise radical pathway involving fast hydrogen atom abstraction followed by radical rebound. Plausible origin of extremely high turnover numbers along with air-compatibility was also rationalized by experiments and DFT calculations.

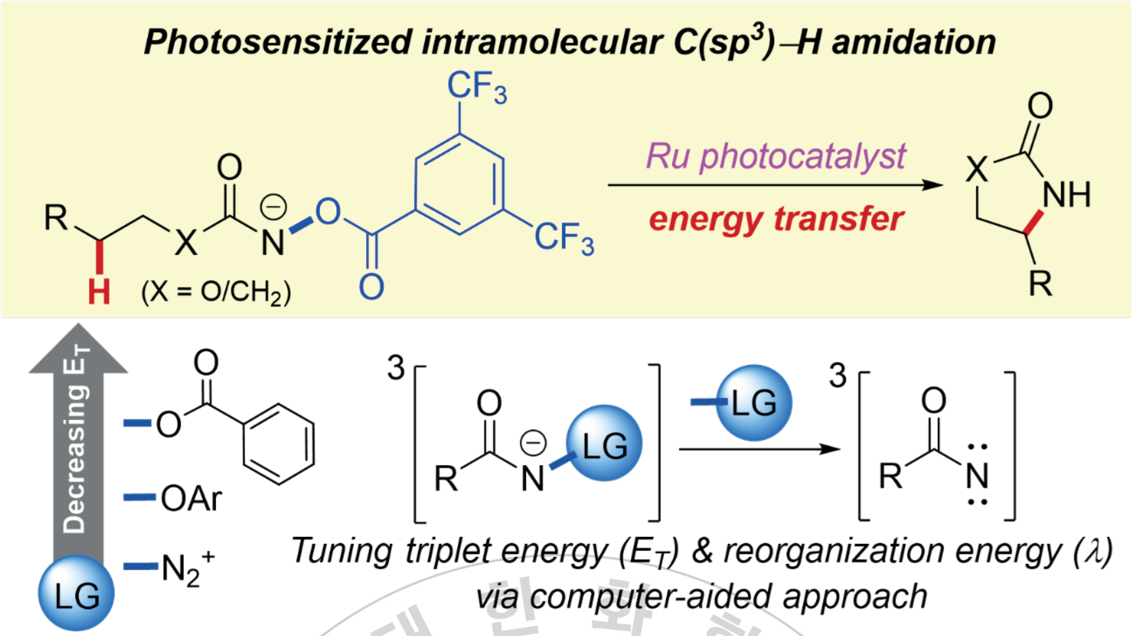
Poster Presentation : **ORGN.P-434**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Visible-Light Photocatalysis of Hydroxamates for Intramolecular C–H Amidation

Hoimin Jung, Hyeyun Keum, Jeonguk Kweon, Sukbok Chang*

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

Nitrogen-centered reactive intermediates such as amidyl radicals and nitrenes have attracted increasing interest mainly due to their potential applicability in the construction of C–N bonds. In this context, we designed a photosensitization strategy to generate triplet nitrenes and applied it for the intramolecular C–H amidation reactions. Substrate optimization by tuning triplet energy led us to identify hydroxamates as potent nitrene sources. While organic azidoformates, which are more classical nitrene sources, were ineffective under the current photosensitization conditions, hydroxamates, which are readily available from alcohols or carboxylic acids, are highly effective in accessing synthetically valuable 2-oxazolidinones and γ-lactams by visible light. Experimental mechanism studies supported our working hypothesis that the energy transfer path is mainly operative.


Photosensitized intramolecular C(sp3)–H amidation
CF3
O
R
X
N
O
H
(X = O/CH2)
O
CF3
Ru photocatalyst
energy transfer
O
X
NH
R
Decreasing ET
O
O
OAr
N2+
LG
3
O
R
N
LG
LG
3
O
R
N
Tuning triplet energy (ET) & reorganization energy (λ)
via computer-aided approach

Poster Presentation : **ORGN.P-435**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

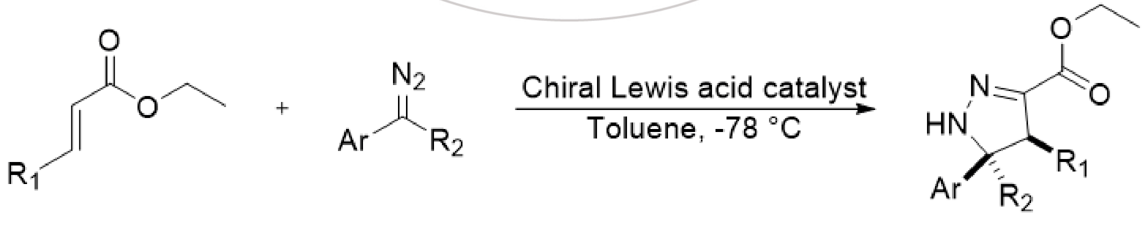
Catalytic Enantioselective 1,3-Dipolar Cycloadditions : Synthesis of 2-Pyrazolines Using Chiral Boron-Based Lewis Acid

Kyung Yee Park, Do Hyun Ryu[1,*]

Chemistry, Sungkyunkwan University, Korea

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

Many natural products and artificial compounds[1] with nitrogen-containing rings are easily found. Especially, various chiral pyrazolines are important core structures for synthesis of many pharmaceuticals, so they have been researched and synthesized through several methods such as using transition-metal catalysis[2] or radical chemistry[3]. In this work, our research group synthesized chiral 2-pyrazolines with excellent yields(up to 99%) and enantioselectivities(up to >99%) through enantioselective 1,3-dipolar cycloadditions from *α*, *β*-unsaturated ester and diazo compounds using boron-based chiral Lewis acid catalyst.References1. Remen L.; Benzençon O.; Simons L.; Gaston R.; Downing D.; Gatfield J.; Roch C.; Kessler M.; Mosbacher J.; Pfeifer T.; Grisostomi C.; Rey M.; Ertel E. A.; Moon R. *J. Med. Chem.* **2016**, *59*, 83982. Kano T.; Hashimoto T.; Maruoka K. *J. Am. Chem. Soc.* **2006**, *128*, 21743. Su Y.; Dong K.; Zheng H.; Doyle M. P. *Angew. Chem. Int. Ed.* **2021**, *60*, 1



yield up to 99%
ee up to >99%

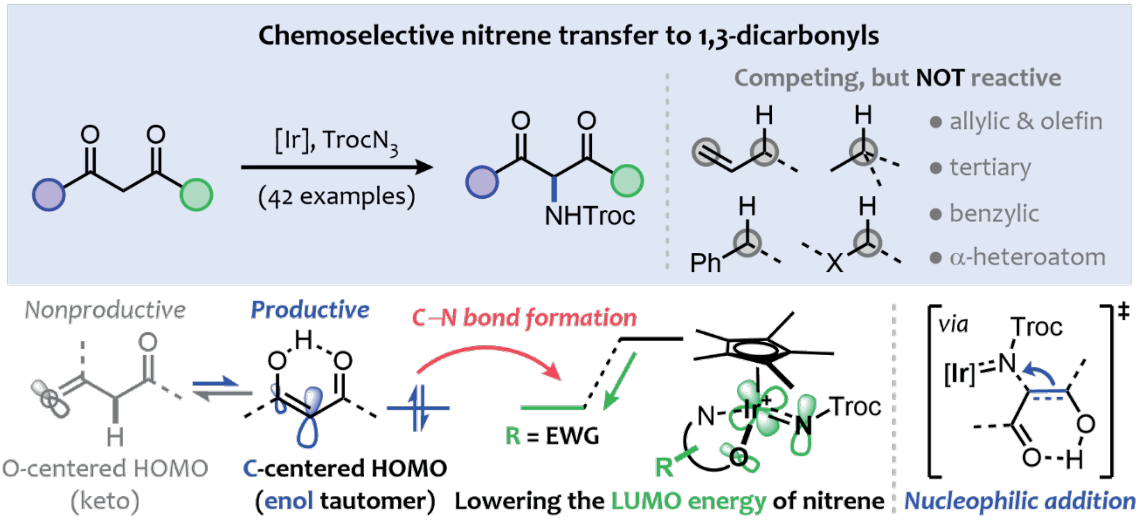
Poster Presentation : **ORGN.P-436**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Modular Tuning of Electrophilic Reactivity of Iridium Nitrenoids for the Intermolecular Selective α-Amidation of β-Keto Esters: A New Way to Make α-Aminocarbonyls

Minhan Lee, Hoimin Jung, Dongwook Kim[1], Jung-Woo Park[2,*], Sukbok Chang[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*
[2]*Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, Korea*

The α-amination of carbonyl compounds has received great interest in synthetic and medicinal chemistry as a straightforward route to versatile building units widely present in natural products and pharmaceuticals. Since the α-carbonyl carbon and amine reactants are electronically mismatched, a polarity reversal of reaction components is required to enable a C–N bond formation at this α-position. In this context, while electrophilic amination has been well-established, the currently available α-amination relies on the use of pre-generated enolates, enamines, or β-keto carbonyls bearing activated methylene sites to react with contrived N-electrophiles such as azodicarboxylates, nitroso reactants, or sulfonyliminoiodinane. However, directly transferring an amino group to the α-position of carbonyls via a metal-nitrenoid intermediate could be a viable alternative. Continuing our efforts on utilizing the reactivity of metal-nitrenoids toward challenging C–N bond-forming processes, we envisioned to achieve selective α-amidation of 1,3-dicarbonyl compounds via an intermolecular carbonylnitrene transfer by modulating electrophilicity of the key intermediate. To this end, we hypothesized that LUMO energy of the presupposed Cp*Ir-nitrenoid can be tuned to enhance its electrophilicity through the bidentate chelating ligand. In particular, when β-keto esters (amides) are of interest, we envisaged that HOMO located at the C=C π-bond of an enol tautomer would efficiently interact with the engineered LUMO of metal-nitrenoid to facilitate an intermolecular C–N bond formation. This closed-shell platform was projected to offer distinctive chemoselectivity toward the α-carbonyl amidation even in the presence of competing reactive sites.


Chemoselective nitrene transfer to 1,3-dicarbonyls
[Ir], TrocN3
(42 examples)
NHTroc
Competing, but NOT reactive
allylic & olefin
tertiary
benzylic
α-heteroatom
Ph
X
Nonproductive
O-centered HOMO
(keto)
Productive
C-centered HOMO
(enol tautomer)
C–N bond formation
R = EWG
Troc
Lowering the LUMO energy of nitrene
via
[Ir]
Nucleophilic addition

Poster Presentation : **ORGN.P-437**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthetic Studies on Functionalized Bridged Oxabicycles via Prin-type Cyclization

Do Hoon Cha, Sun-Joon Min[1,*]

Department of Applied chemistry, Hanyang University, Korea
[1]*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

Bridged Oxabicycle is a molecular scaffold that consists of the two joined rings sharing three or more atoms, separating the two bridgehead atoms by a bridge containing oxygen. This structural feature is frequently found in various biologically important natural products such as englerin, cortistatin, balsmiferine and so on. For example, englerin, a sesquiterpene isolated from the bark of euphorbiaceae Phyllanthus engleri, exhibits significant anti-cancer activity, especially for renal cell carcinoma. Cortistatin is a steroidal alkaloid isolated from the marine sponge Corticium simplex, which inhibits proliferation of human umbilical vein endothelial cells. Although the synthetic approaches toward this molecular architecture have been studied, the stereoselective construction of bridged oxabicycle system is still challenging to synthetic organic chemists due to its complexity and application to total synthesis.Herein, we report our efforts to synthesize functionalized bridged oxabicycles via Prins-type cyclization of vinyl spirolactol. The key feature of this presentation includes stereospecific ring opening of epoxide, stereoselective Grignard reactions and reaction optimization of Prins-type cyclication.

Poster Presentation : **ORGN.P-438**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Design and synthesis of battery electrolyte additives with dioxolone derivatives for lithium-ion batteries

SeoYoung Jeong, Sung You Hong*

Chemistry, Ulsan National Institute of Science and Technology, Korea

Vinylene carbonate (VC) derivatives are very significant structure in the field of electrolyte additives for Li-ion battery. VC derivatives could form a stable SEI, which could prevent electrolyte degradation by blocking the electron transport while allowing lithium ions to pass during cycling. Electrolyte additives are the most economical and efficient method to solve theses problems and thus improve lithium ion battery performance. However, current conventional solid electrolyte interphase additives, such as vinylene carbonate and fluoroethylene carbonate, have limitations of abilities of achieving a long lifespan and fast chargeability in lithium-ion batteries (LIBs) for simultaneously. Here we reported a next-generation synthetic additive with dioxolonee. In terms of syntesis, O-trifluoromethylation has been a challenging task in organic synthesis. We installed CF3 and TMS group to alcohol via the modified method from the precedent protocols appropriately.The retrosynthetically designed solid electrolyte interphase-forming additives, 5-methyl-4-((trifluoromethoxy)methyl)-1,3-dioxol-2-one and 5-methyl-4-((trimethylsilyloxy)methyl)-1,3-dioxol-2-one can form highly stable interface. The interface architecture from the synthesized vinylene carbonate-type additive enables high-energy-density LIBs with 81.5% capacity retention after 400 cycles at 1 C and fast charging capability (1.9% capacity fading after 100 cycles at 3 C).

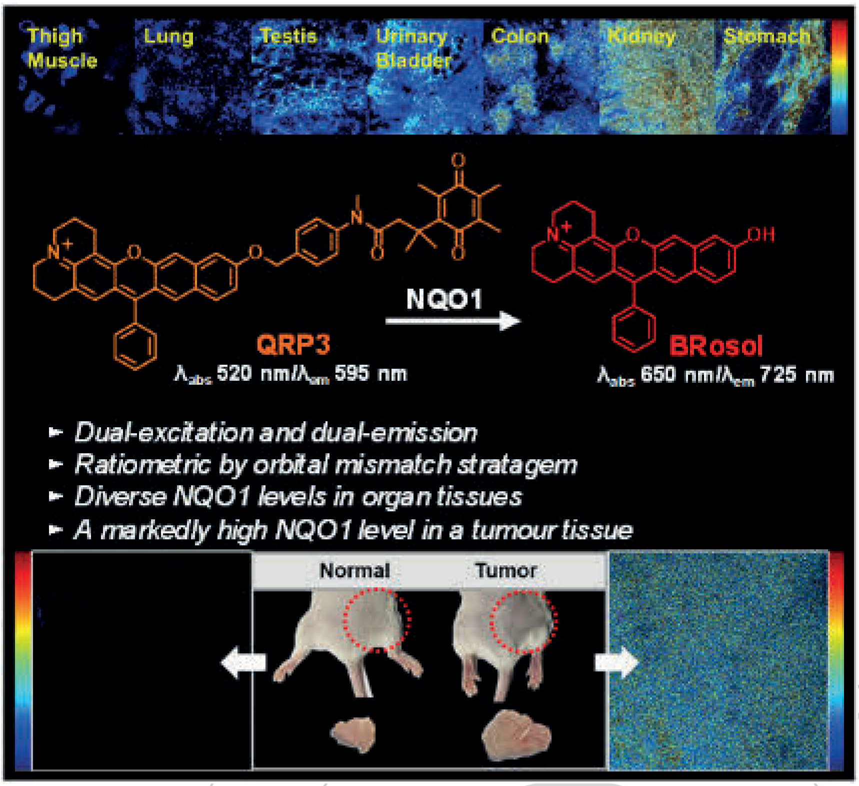
Poster Presentation : **ORGN.P-439**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Benzorosol-Based Dual-Excitation and Dual-Emission Probe: Quantitative Fluorescence Imaging of NAD(P)H Quinone Oxidoreductase-1 in Organ and Tumor Tissues

Yun Jae Yang, **Kyo Han Ahn***

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

NAD(P)H quinone oxidoreductase-1 (NQO1) plays important roles in biological system such as chemoprotecting/detoxifying of quinones, scavenging of superoxide, stabilizing of tumor suppressors, and maintaining endogenous antioxidants under cellular oxidative stress.[1] And as a dark side, a high expression level of NQO1 is associated with chemoresistance of cancer. Accordingly, abnormally high expression of NQO1 in solid tumor is the standard of cancer biomarker. For practical development of probe, four candidates were prepared through introduction of the quinone moiety known as the enzyme-reactive substrate to benzo-rosol fluorophores. According to the computational study and photophysical study, four candidates can be applied as ratiometric probes based on orbital mismatch strategy with intramolecular charge transfer mechanism. Notably, one ether-linked probe with self-immolative linker shows high stability and fluorescent brightness in cellular condition. We further applied probe for measuring the NQO1 activity levels in several organ tissue. Furthermore, probe showed 14.6 folds higher signal in the xenograft tissue compared with the normal tissue and offers important means as a practical tool for cancer diagnosis and NQO1-associated biology.[2] Reference1.D. Ross, D. Siegel, *Front. Physiol.* **2017**, *8*, https://doi.org/10.3389/fphys.2017.005952. Y. J. Yang, M. Dai, Y. J. Reo, C.W. Song, S. Sarkar and K. H. Ahn, *Anal. Chem.* **2021**, *93*, 7523



- *Dual-excitation and dual-emission*
- *Ratiometric by orbital mismatch stratagem*
- *Diverse NQO1 levels in organ tissues*
- *A markedly high NQO1 level in a tumour tissue*

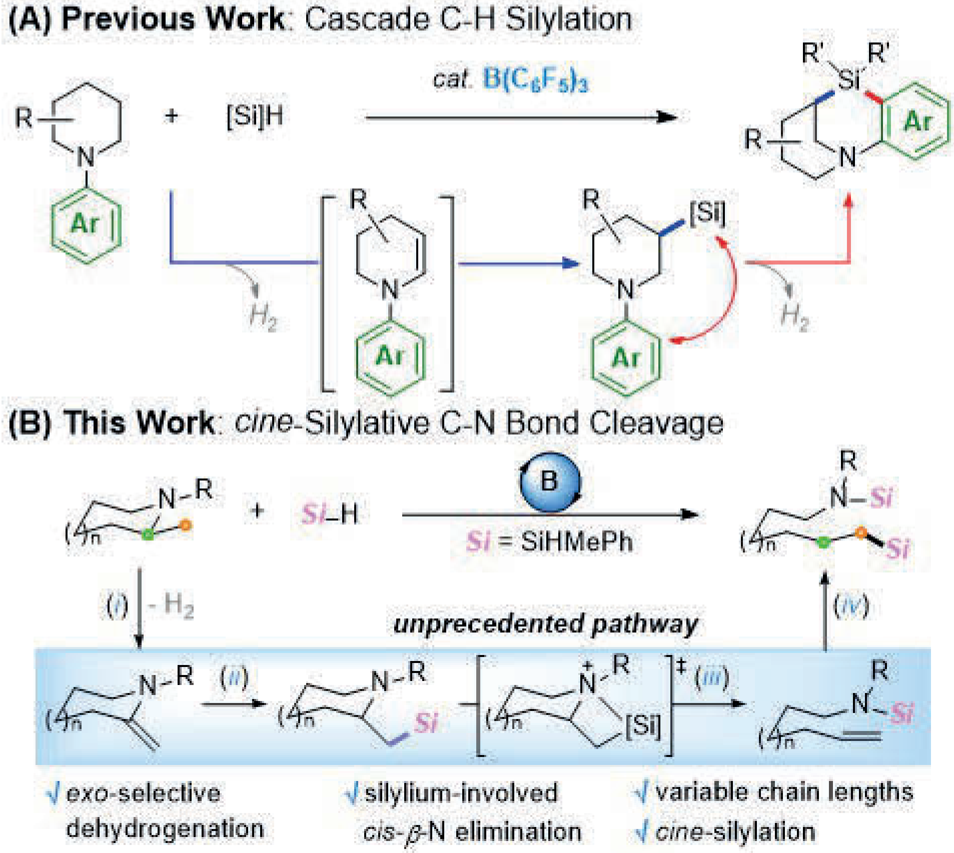
Poster Presentation : **ORGN.P-440**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

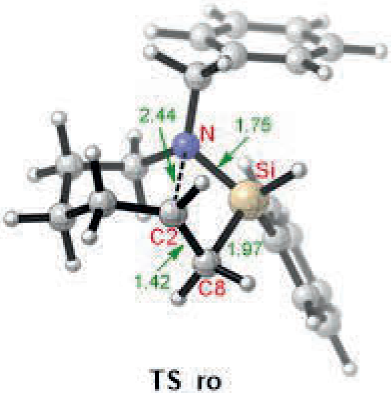
Borane-Catalyzed C-N Bond Cleavage Enabled by Silylium-Induced beta-Nitrogen Elimination

Jianbo Zhang, Sukbok Chang[1,*]

Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, Korea
[1]*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Site-selective modifications of azacycles with transition metal catalysis has emerged as a powerful tool with the assistance of directing groups while the approaches based on organocatalyst are often limited in scope. Our group previously showed that $B(C_6F_5)_3$-catalyzed a cascade process of beta-silylation of N-arylpiperidines via enamine intermediates. As a complementary strategy, the deconstructive functionalization of N-heterocycles has also drawn an increas-ing interest in recent years. This approach provides acyclic amines tethered with remote functional groups. An unprecedented borane-catalyzed *cine*-silylative ring-opening of alph-methyl azacycles is achieved, involving four-step cascade processes: (i) *exo*-dehydrogenation of alicyclic amine, (ii) hydrosilylation of resultant enamine, (iii) silylium-induced *cis*-beta-amino elimination to open the ring skeleton, and (iv) hydrosilylation of terminal olefin. The present borane catalysis also works efficiently for the C–N bond cleavage of acyclic tertiary amines. On the basis of experimental and computational studies, the silicon atom was elucidated to play a pivotal role in the beta-amino elimination step. The procedure is readily expanded to the C-N bond cleavage of acyclic tertiary amines.





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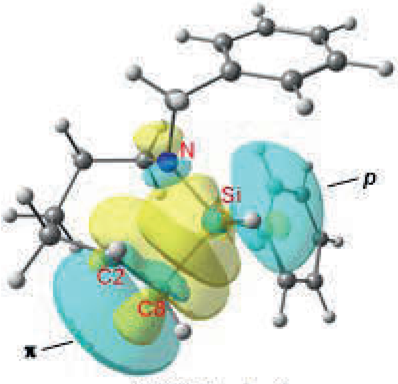


NBO Analysis

Poster Presentation : **ORGN.P-441**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A ratiometric fluorescent sensor based on host-guest interaction of self-assembled pyrenyl-nanofibrils with γ-cyclodextrin for detection of α-amylase activity in urine

Tae Min Park, Su Jin Na, Minwoo Han, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

In this study, an effective fluorescent biosensor was developed for quantitative detection of α-amylase activity based on host-guest interaction between self-assembled pyrenyl-nanofibrils and γ-cyclodextrin (γ-CD). The amphiphilic pyrenyl derivatives form the self-assembled nanofibrils in aqueous media. Their monomeric components are captured by γ-CD and forms a dimer of the Py-CO2:γ-CD complex. After that, the γ-CD is decomposed by amylase, indicating that nanofibril is re-formed. Furthermore, this sensing platform has been successfully utilized to monitor α-amylase at very low concentration in urine, which shows potential in relevant clinical diagnostics.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **ORGN.P-442**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Protamine-induced supramolecular self-assembly of TPE derivatives for sensitive detection of trypsin activity

HyeBin Song, Haemin Choi, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

A New fluorescence strategy is developed based on protamine-induced supramolecular self-assembly of tetraphenylethylene (TPE) derivatives with water-soluble pendants for the efficient detection of trypsin activity. Protamine induces supramolecular self-assembly of water-soluble TPE derivatives by electrostatic interaction and π–π stacking, resulting in a drastic fluorescence enhancement via aggregation induced emission (AIE). This system can efficiently detect the activity of trypsin, which can degrade TPE aggregation by hydrolysis of protamine into fragments. This study has proven to be a sensitive and selective detection method not only for trypsin, but also for the screening of trypsin inhibitors, which are essential for the discovery of new drugs.

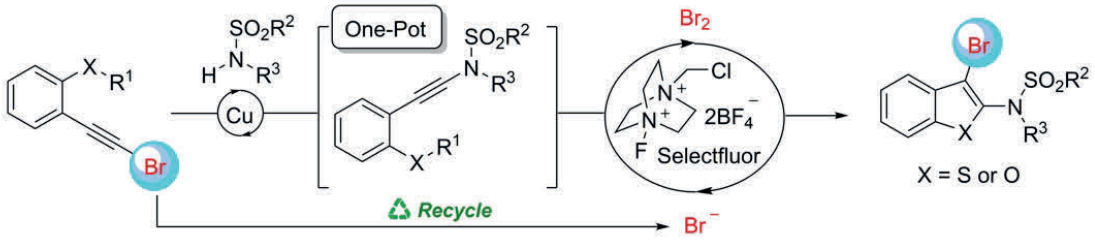
Poster Presentation : **ORGN.P-443**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Economical route to 2-amido-3-bromobenzo[*b*]thiophenes *via* ynamide formation and Selectfluor-mediated oxidative bromocyclization

SuJeong Hong, **Hee Nam Lim**[1,*], **Hyun-Suk Yeom**[2,*]

Korea Research Institute of Chemical Technology, Korea
[1]*Department of Chemistry and Biochemistry, Yeungnam University, Korea*
[2]*Center for Eco-Friendly New Materials, Korea Research Institute of Chemical Technology, Korea*

Benzo[*b*]thiophenes are biologically important scaffold that have been widely studied in medicinal chemistry field. Thus, Synthesis of benzo[*b*]thiophenes has attracted great attention over the past few decades. In particular, 3-halogenated benzo[*b*]thiophene is easy to structurally expand thought substitution and cross coupling(C-C or C-N) reactions. Recently, Our group has been developed a one-pot synthesis of 2-amido-3-bromobenzo[*b*]thiophenes based on C-N coupling and oxidative bromocyclization reactions. This method enables a modular approach to obtain diverse sulfonamide substituents at the C2 position of benzo[*b*]thiophene also introduce Br atom at the C3 position through recycling of Bromo anion generated in the C-N bond coupling step. Oxidative cyclization was driven by Selectfluor and represents a previously unreported recycling method for the bromide anion. The details of the study are described in this presentation.



Poster Presentation : **ORGN.P-444**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Conformation and Permeability Study of Hydroxyl Side Chain-containing Cyclosporin O Derivatives

Namhee Kim, Jiwon Seo[1,*]

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

For intracellular PPI targeting drug, membrane permeability is a critical property. In general, cyclic peptides have lower membrane permeability than small molecules due to their larger size. Also, incorporation of polar side chain into a cyclic peptide gives variation on lipophilicity and intramolecular hydrogen bonding which changes for its permeability and conformational homogeneity. Here, we designed polar residue containing cyclic peptides using cyclosporin O (CsO), natural macrocyclic peptide, as a scaffold. Synthesized cyclic peptides showed its conformational homogeneity by NMR spectroscopy and its membrane permeability by parallel artificial membrane permeability assay (PAMPA). We found that D-amino acid position substituted peptide did not show significant decrease in permeability compared to CsO. In addition, the following peptide exhibited 3-fold increase in permeability than the other position substitution. This result suggests that CsO scaffold is tolerable to tyrosine in terms of the maintenance of membrane permeability. In our study, effect of polar residue incorporation to CsO and importance of the position of polar residue in CsO were shown. With further conformation study, this permeability tolerance trend is expected to be explained.

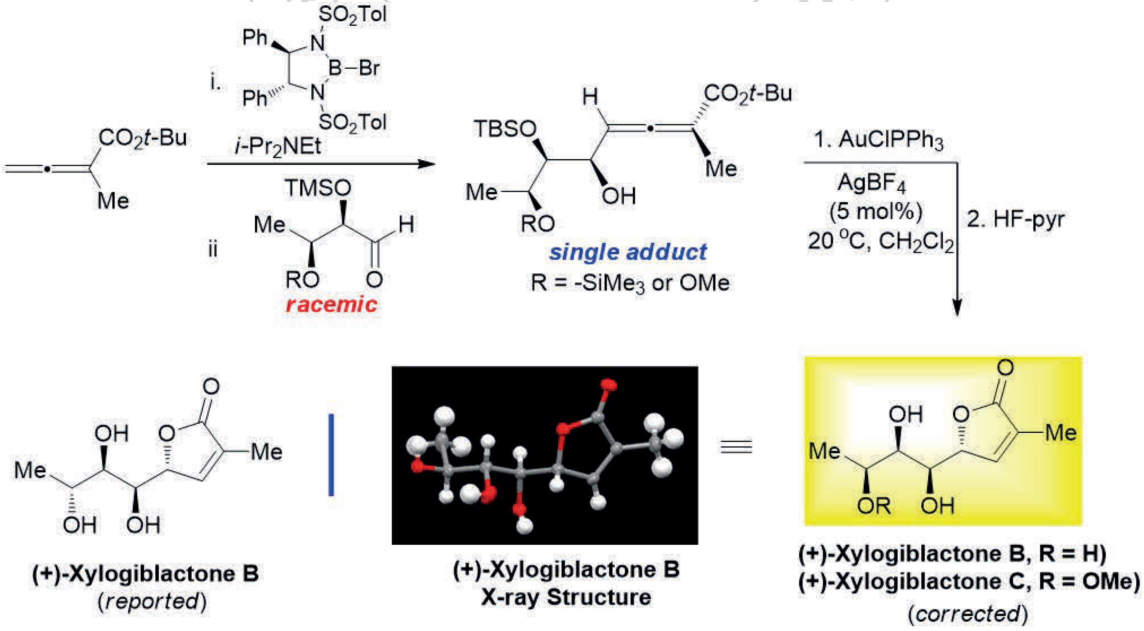
Poster Presentation : **ORGN.P-445**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Revision of Stereochemistry for Xylogiblactone B and C through Asymmetric Allenoate Gamma-addition

Zhang Aimin, Euijin Park, Jimin Kim*, Hyeonjoung Choi

Department of Chemistry, Chonnam National University, Korea

Synthesis of natural butenolide (+)-xylogiblactone B was achieved in linear 3 steps from the allenoate. Kinetic resolution of racemic aldehyde through the allenoate g-addition at –20 oC to afford g-adduct as a single regio- and stereo isomer. Regiospecfic cyclization of g-adduct via gold catalysis using Ph3PAuNTf2 (10mol%) provided the g-butenolide core. Acidic deprotection of silyl groups afforded (+)-xylogiblactone B as a stereochemically pure form. Stereochemical relationship of the reported structure of (+)-xylogiblactone B was corrected based on analysis of x-ray crystal structures of the synthetic intermediates and the product. We believe that chemical synthesis still has important roles to play in the process of solving molecular architecture.



Poster Presentation : **ORGN.P-446**

Organic Chemistry

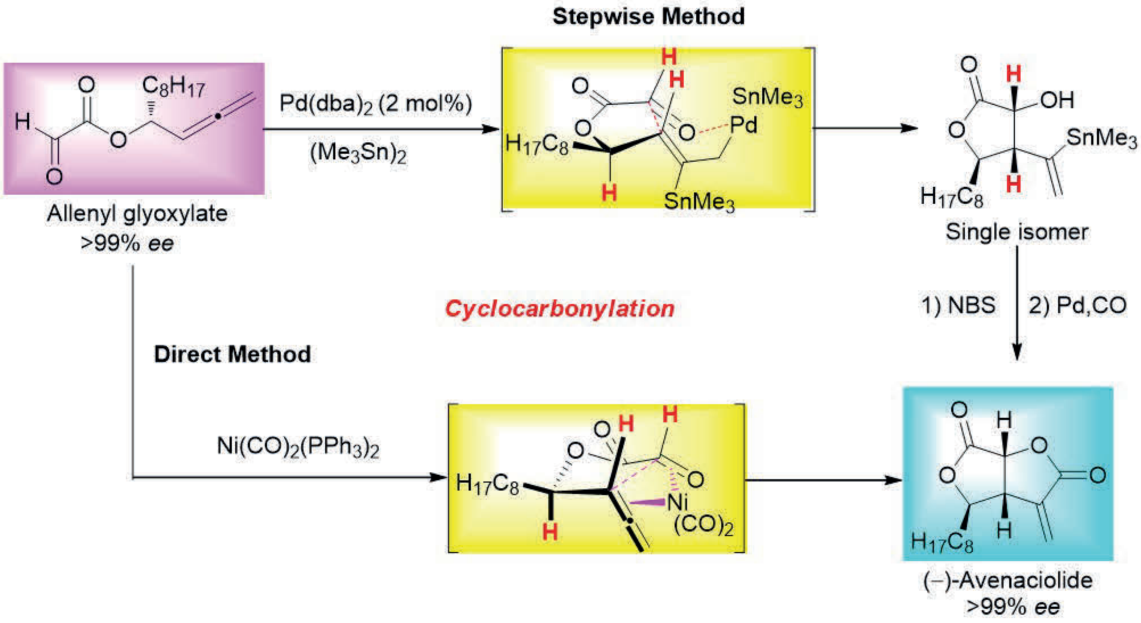
Exhibition Hall 1 FRI 11:00~12:30

Enantioselective Synthesis of (-)-Avenaciolide from Allenyl Glyoxylate via Direct and Stepwise Cyclocarbonylation

Zhang Aimin, **Sehui Yang, Suh Young Yu, Jimin Kim**[*]

Department of Chemistry, Chonnam National University, Korea

Development of new synthetic protocols for achieving a stereoselective construction of a highly functionalized bicyclic system is a valuable objective owing to the presence of this core unit in many natural products including (-)-avenaciolide possessing a diverse array of biological activities. We would like to present herein several crucial points that have emerged during our recent investigations for the synthesis of naturally occurring (-)-avenaciolide: i. Optimization of reaction conditions for direct and stepwise cyclocarbonylation processes via transition metal catalysis. ii. Chemical conversions through functional group transformations for the synthesis of target molecule.



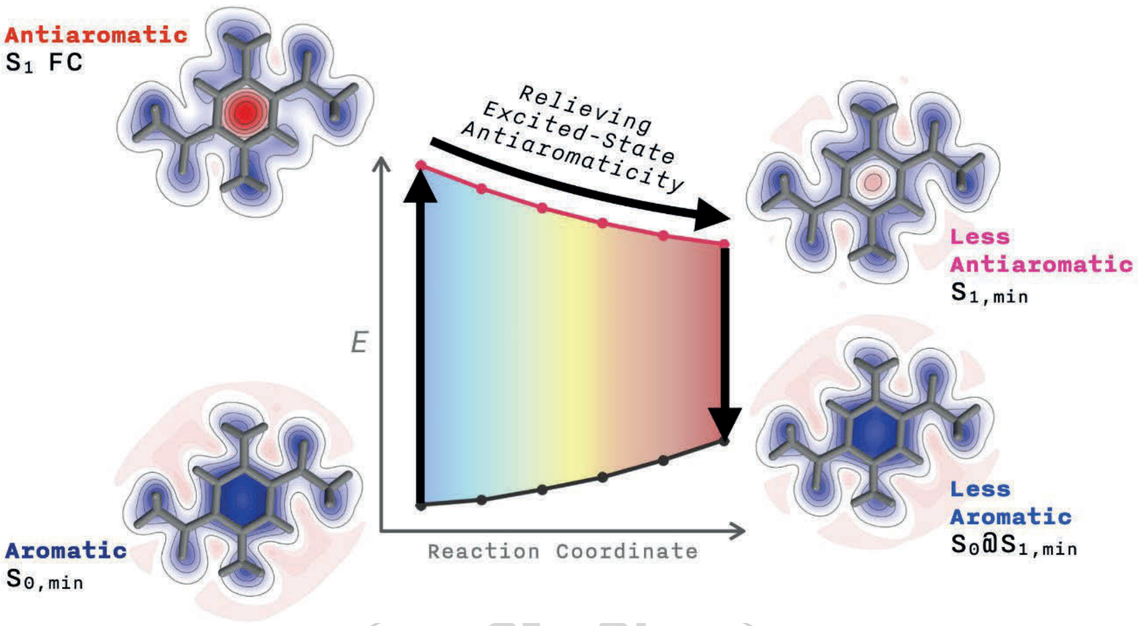
Poster Presentation : **ORGN.P-447**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

The Lightest Red Emitter: Electronic Origin of Large Spectral Shift and Structural Diversification into Full-Color Single-Benzene Fluorophores

Heechan Kim, Younghun Kim, Woojin Park[1], Cheol Ho Choi[1,*], Dongwhan Lee[*]

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

Existing strategies to achieve large Stokes shifts rely on appending peripheral groups to known fluorophores, but often compromise other photophysical properties such as emission wavelength and quantum yield. The development of small fluorogenic motif exhibiting large Stokes shift is an unsolved and challenging problem. We disclose a new class of tunable light-emitters based on a simple benzene core. Among the three regioisomers of DAPAs (diacetylphenylenediamines), *o*- and *p*-DAPA are fluorescent, whereas *m*-DAPA is not. Remarkably, *p*-DAPA is the lightest (FW = 192) molecule ever known that displays red emission ($\lambda_{\mathrm{em,max}}$ > 600 nm). Late-stage single-step modification of the parent *p*-DAPA platform afforded a library of fluorophores covering the entire visible spectral window. The electronic origin of this intriguing structure–property relationship was unveiled by in-depth theoretical studies on the excited-state dynamics and reaction coordinates. We found that the large Stokes shifts of DAPA fluorophores originate from the relief of antiaromaticity in the excited-state of the benzene core, rather than the typically assumed charge-transfer or proton transfer involving peripheral groups. This presentation will discuss a new strategy to develop single benzene fluorophores with long-wavelength light emission, without the need for large and extended π-conjugation.


Antiaromatic
S1 FC
Relieving Excited-State Antiaromaticity
Less Antiaromatic
S1,min
E
Aromatic
S0,min
Less Aromatic
S0@S1,min
Reaction Coordinate

Poster Presentation : **ORGN.P-448**

Organic Chemistry

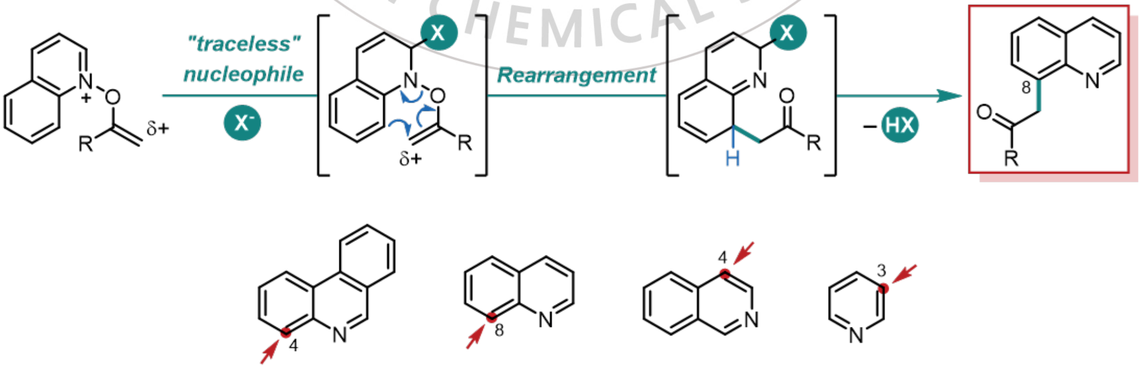
Exhibition Hall 1 FRI 11:00~12:30

Siteselective C–H Functionalization of Heteroarene *N*-Oxides using a Traceless Nucleophile

Byeongseok Kweon, Sungwoo Hong*

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

Although *N*-alkenoxyheteroarenium salts have been widely used as umpoled synthons with nucleophilic heteroarenes, the use of electron-poor heteroarenes has remained unexplored. To overcome the inherent electron deficiency of quinolinium salts, a traceless nucleophile-triggered strategy was designed, wherein the quinolinium segment is converted into a dearomatized intermediate, thereby allowing simultaneous C8-functionalization of quinolines at room temperature. Experimental and computational studies support the traceless operation of a nucleophile, which enables the previously inaccessible transformation of *N*-alkenoxyheteroarenium salts. Remarkably, the generality of this strategy has been further demonstrated by broad applications in the regioselective C–H functionalization of other electron-deficient heteroarenes such as phenanthridine, isoquinoline, and pyridine *N*-oxides, offering a practical tool for the late-stage functionalization of complex biorelevant molecules.



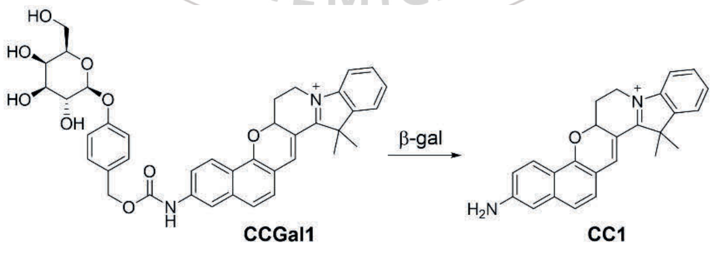
Poster Presentation : **ORGN.P-449**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Highly Stable Red-Emissive Ratiometric Sensor for Monitoring of β-galactosidase Activity in Cancer Models

Hyo Won Lee, Hwan Myung Kim[1,*]

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

β-galactosidase (β-gal), well-known as a useful reporter enzyme, is an effective biomarker for various diseases such as colorectal and ovarian cancers. In this study, we have developed a highly stable red-emissive ratiometric fluorescent sensor (CCGal1) for quantitative monitoring of β-gal enzyme activity in live samples. This ratiometric sensor exhibited rapid emission color change (620 to 662 nm) in response to β-gal sensitively and selectively, which accompanied high enzyme reaction efficiency, cell-loading ability, and remarkable stability with negligible cytotoxicity. Confocal fluorescence microscopy ratiometric images, with the combination of fluorescence-activated cell sorting (FACS) flow cytometry, revealed that CCGal1 could provide useful information to diagnose, prognose, and therapy of β-gal enzyme activity-associated diseases such as colorectal, and ovarian cancers. Moreover, it may yield meaningful strategies for designing and modifying multifunctional bio-sensors with different biomedical applications.



Scheme 1. Chemical structures of **CCGal1** and the corresponding hydrolysed product (**CC1**).

Poster Presentation : **ORGN.P-450**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Cancer selective azo dyes using two-photon photodynamic therapy in human colon tissue

DongJoon Lee, Hwan Myung Kim[1,*]

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

Inappropriate cancer control can be prevented by simultaneous cancer diagnosis, treatment, and real-time assessment of therapeutic processes. Here we report the design of the two-photon (TP) photosensitiser (PS), ACC-B, for high temporal and spatially selective near-infrared cancer therapy. ACC-B consisting of a biotin unit remarkably enhanced the cancer sensitivity of the PS. Upon TP irradiation, ACC-B generated reactive oxygen species by type I photodynamic therapy (PDT) process and triggered highly selective cancer ablation. In addition, TP microscopic images showed significant differences in ACC-B uptake between normal and cancerous tissues in living human colon tissue, and this property was used for real-time imaging. Also, ACC-B generated ROS efficiently in live colon cancer tissues with high spatial selectivity. During PDT, ACC-B can provide in situ spatioselective visualization of cellular behaviour and molecular information for therapeutic assessment in specific regions.

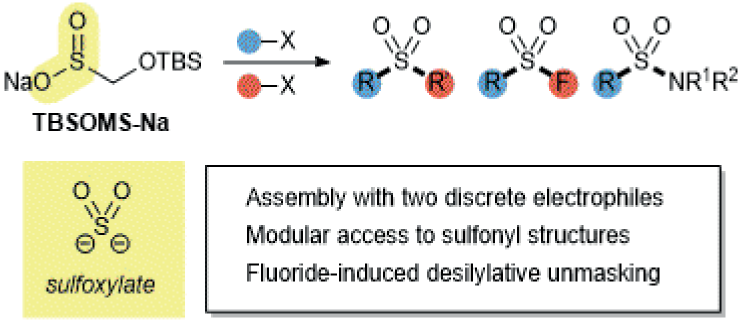
Poster Presentation : **ORGN.P-451**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Silyloxymethanesulfinate as a sulfoxylate equivalent for the modular synthesis of sulfones and sulfonyl derivatives

Dae-Kwon Kim, Hyun-Suk Um, Chulbom Lee*

Division of Chemistry, Seoul National University, Korea

Sulfonyl units ($–SO_2^–$) occur in many useful organic molecules such as sulfones, sulfonamides and sulfonyl fluorides. Traditionally, their preparation has largely been dependent on oxidizing the sulfur atom in sulfides derived from thiols, which pose handling problems due to their foul odor. In this context sulfur dioxide surrogates have provided useful means for direct introduction of sulfonyl motifs under simple and mild conditions. We explored the use of the novel sulfinate reagent, **TBSOMS-Na**, from Rongalite™, previously developed for stereoselective allylic reduction via liberation of sulfur dioxide,[1] for installation of sulfonyl motifs into organic molecules. As a dianion equivalent of sulfur dioxide, sulfoxylate ($SO_2^{2–}$) has the potential for the construction of a wide range of structures by joining with two electrophiles. Recent reports have also disclosed the conceptual demonstration of Rongalite™ or its derivative as a sulfoxylate equivalent. However, the structural variety of accessible sulfones is limited. In contrast, TBSOMS-Na is found to be able to react with aryl and alkyl electrophiles to form the stable sulfone intermediate, which can generate a new sulfinate ready for additional alkylation or arylation. Coupling with various aryl electrophiles as well as other functionalization reactions can be carried out with orthogonal unmasking in a single operation. Our studies have shown that TBSOMS-Na, a bench-stable sulfinate reagent, is widely applicable in the synthesis of sulfones and sulfonyl derivatives.



Assembly with two discrete electrophiles
Modular access to sulfonyl structures
Fluoride-induced desilylative unmasking

Poster Presentation : **ORGN.P-452**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A two-photon mitochondrial sodium ion sensor for live tissue imaging

Vinayak Juvekar, Hwan Myung Kim[1,*]

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

Sodium (Na^+) ions directly influences various cellular functions. Intracellular Na^+ dysregulation due to an imbalance of Na^+ influx and efflux can contribute to serious disorders. Two-photon (TP) fluorescence technology is the most useful non-invasive technique to detect bio-analytes deep within tissues with high spatioselectivity. Therefore, a biocompatible and a bright red emissive TP-probe distinguishing sodium ion imbalance in live specimen can benefit in understanding several biochemical processes influenced by sodium ion homeostasis. Herein, we describe a highly sensitive cyclocyanine-based red-emissive TP probe to detect to detect sodium ions. The developed probe is the first Na^+ ion TP sensor for mitochondria with bright and long-fluorescence emissions. The probe showed significantly different TP action cross section values in the absence and presence of Na^+ ions, respectively. The insensitivity of probe toward solvent polarity and narrow fluorescence spectrum within cells can detect multiple metal ion activity through dual- or multi-color imaging. The probe exhibited easy cell loading, good biocompatibility, and could highlight endogenous mitochondrial Na^+ ions through bright TPM images in mouse hippocampal tissue with negligible interference from other biologically relevant metal ions.

Poster Presentation : **ORGN.P-453**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Dithiolane containing amino acid as a reversible labeling handle

Jeongeun Lee, Minseob Koh*

Department of Chemistry, Pusan National University, Korea

We are devising a system to reversibly label a surface protein of living bacteria. We have developed a dithiolane containing amino acid (dtF) that can be genetically encoded with a help of the selected variant of *Methanocaldococcus jannaschii* tyrosyl-tRNA synthetase/tRNA pair in *Escherichia coli* (*E. coli*) host.[1,2] For an initial proof-of-concept experiment, small molecule labeling was tested at the protein level. The specific site (Y151) of super-folder green fluorescent protein (sfGFP) was mutated to an amber codon (TAG), then dtF was incorporated at the Y151 site. The sfGFP-Y151dtF and the corresponding reduced form (M+2H) in dithiothreitol condition were confirmed by mass spectrometry. To assess whether the dtF incorporated protein can be labeled by a small molecule, we have treated the sfGFP-Y151dtF with a trivalent arsenous acid[3,4]. The protein-small molecule adduct was successfully generated and the reverse reaction was proceeded by treating ethanedithiol. We will further apply this strategy to the surface protein of *E. coli* by targeting an outer membrane protein. In addition, we aim to utilize this strategy for dynamic control of cellular behavior as well as bioimaging.

Poster Presentation : **ORGN.P-454**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Cyanoformates via DAST-mediated Beckmann Fragmentation

Sung Pyo Youn, Hee Nam Lim[1,*]

Chemistry, Yeungnam University, Korea
[1]*Department of Chemistry and Biochemistry, Yeungnam University, Korea*

Cyanoformates are useful chemicals for ketone α-acylation that can lead the selective C-acylation over competing O-acylation. Although conventional synthetic methods for the cyanoformates are established in the industrial process, the drawbacks such as toxicity and limited reagent source remain challenges to overcome. Here, we wish to report a new approach for cyanoformates; the method is based on DAST-mediated C–C bond cleavage of α-oximino-β-ketoesters. Due to simplicity and mildness of the procedure, the method is greatly workable on both small and large scale reactions.

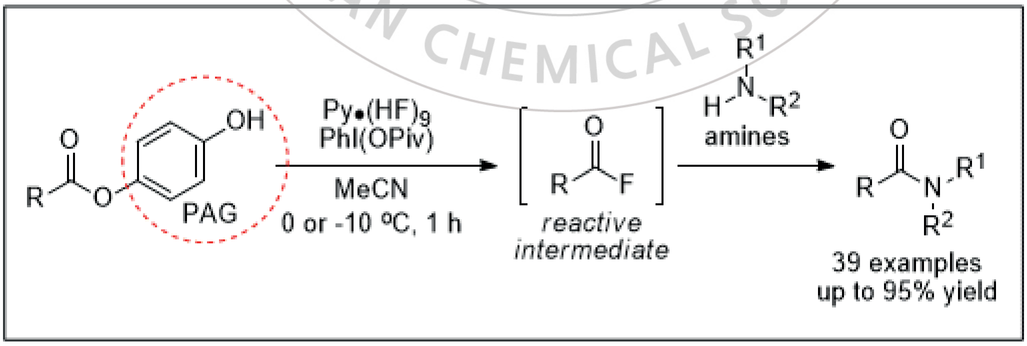
Poster Presentation : **ORGN.P-455**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Amide-bond formation by activation of ester with hypervalent iodine(III) reagent

Eunsol Choi, Hyo-Jun Lee*

Department of Chemistry, Kunsan National University, Korea

Amide bond is the most fundamental functional group in chemistry and found in various bio-active compounds, materials with specific properties, and DNA as well. Therefore, development of efficient method for amide bond formation in mild conditions has been a great interest in organic chemistry. Here, we report a new amide bond formation from esters that possess a phenol moiety as a potential activating group (PAG). The PAG is activated by hypervalent iodine(III) reagent under mild conditions and reactive acyl fluorides intermediate is generated using pyridine hydrogen fluoride complex. Subsequent acyl substitution with amines provides corresponding amides and peptides, including sterically hindered structure in high yield (up to 95 yield). The mechanism and reaction pathway were confirmed by Gibbs free energy profiles and density functional theory (DFT) calculations.



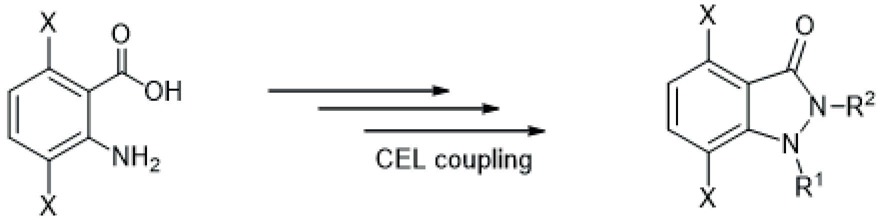
Poster Presentation : **ORGN.P-456**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and biological activity of N2-Arylindazol-3-one derivatives.

Sumin Kim, Hakwon Kim*, Kyungmin Kim, Heejae Choi

Department of Applied Chemistry, Kyung Hee University, Korea

Indazol-3-one, a heterocyclic compound containing benzene and pyrazol-3-one, is well known to exhibit various biological activities.In this study, we synthesized several N2-aryl substituted indazol-3-one derivatives from anthranilic acid. In particular, the N2-ayl substitution reaction of indazol-3-one using CEL (Chan-Evans-Lam) coupling reaction was investigated for the synthesis of N2-aryl-substituted indazol-3-one derivatives. Their biological activity was also investigated.



Poster Presentation : **ORGN.P-457**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Improvement of the reactivity of the acyl azides to synthesize the cyclic acyl amidines

Dong Geun Jo, Seewon Joung[*]

Department of Chemistry, Mokpo National University, Korea

Our previous work has been focused on the development of strategies for the synthesis of cyclic amidines present in a variety of natural and pharmacological molecules. We have reported the synthesis of 6-membered cyclic amidine by utilizing the [3+2] cycloaddition of sulfonyl azide to an enamine intermediate from borane-catalyzed dearomatization of N-heteroarene.In our previous investigations, it was reported that the reaction between the enamine intermediate and the acyl azide did not proceed because acyl azide was less reactive than sulfonyl azide. Although the benzoyl azide and enamine intermediates have shown low reactivity, it was possible to improve the reactivity by attaching functional groups to the benzoyl azide. Herein, we report synthesis of various cyclic acyl amidines from electron withdrawing acyl azides.

Poster Presentation : **ORGN.P-458**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Direct Access to Carbamates via Catalytic Reductive Amination

Woohee Kim, Han Yong Bae*

Department of Chemistry, Sungkyunkwan University, Korea

The alpha-secondary amine is a frequently encountered structural scaffold in a wide variety of natural products and pharmaceuticals. To access this moiety, reductive amination of the ketone is regarded as an inarguably powerful chemical process. Though numerous advancements have been made, a more sustainable method is still highly demanded from the green chemistry perspective. In this regard, when it comes to the chemistry of catalytic hydroboration of unsaturated C=N bond, the utilization of preformed N-aryl or N-alkyl ketimines from starting ketones (C=O) is essential for the successful transformation. However, direct access to the α-secondary amine moiety is entirely unknown; this is perhaps due to the under-controlled strong background reaction between borane and ketone, which end up with reduced secondary alcohol. Here we show the first example of a transition metal-free approach toward synthetically advantageous carbamates which incorporate alpha-secondary amines via Brønsted acid-catalyzed reductive amination. The key to the successful chemoselective transformation was using readily accessible amines, boronic acid pinacol ester, and strong acid catalyst as a compelling combination. The synthetic utilities of the obtained products were applied to the syntheses of a few useful drug intermediates.

Poster Presentation : **ORGN.P-459**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Beta-Sulfido-SuFEx Hubs via Superbase Catalysis “on-Water”

Sunbu Lee, Jin Hyun Park, Han Yong Bae*

Department of Chemistry, Sungkyunkwan University, Korea

Beta-sulfidosulfonyl fluoride moieties are found in a number of important bioactive compounds, e.g., PMPMEase inhibitors, lipoprotein lipase inhibitors, and G-site inhibitors for GSTP1-1. Conventional approaches toward such aliphatic sulfonyl fluorides require a few chemical transformations, including several redox and fluorination steps. Due to these challenges, a good functional group tolerance is rarely guaranteed, thus, a more efficient and readily accessible process is highly demanded. In line with this effort, ethenesulfonyl fluoride (ESF) has recently emerged as a useful building block for the sulfur(VI) fluoride exchange reaction (SuFEx), and is widely utilized to install their key SuFEx Hub. Here we show the first example of a remarkable rate acceleration effect of the thia-Michael addition reaction to afford beta-sulfidosulfonyl fluorides “on-water”. Using PPM-level amount of phosphazene superbase enabled the successful key transformation with high chemo-/site-selectivities, and good functional group tolerance. A wide variety of beta-aryl-substituted ESFs were smoothly converted to the desired thia-Michael products in up to >99% yield. Further useful SuFEx ligations of the obtained product were optimized by taking advantage of the conditional reactivity of the sulfonyl fluorides.

Poster Presentation : **ORGN.P-460**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Organic Photoredox Catalysis for Deaminative Coupling Reactions

Byeong Jun Koo, Han Yong Bae*

Department of Chemistry, Sungkyunkwan University, Korea

Primary amines are ubiquitous organonitrogen compounds frequently encountered in abundant feedstocks, e.g., natural amino acids. Activating such C–N bonds together with simultaneous installation of useful functional groups is one of the most challenging tasks in modern chemical society. Here we show the visible-light-driven photoredox catalysis that enabled deaminative C(sp3)–C(sp3) coupling reactions under the aqueous conditions. The catalyst loading of the discovered organic photosensitizer could be lowered to 0.1 mol% retaining the high chemical yield of desired products. The pre-activation of starting amines to Katritzky pyridinium salts was the key to successful catalysis. The non-innocent aqueous condition could be applied to a wide variety of functionalized alkenes, afforded aliphatic sulfonyl fluorides, nitriles, esters, and boronic acid esters.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **ORGN.P-461**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Ni-catalyzed stereospecific substitution to form quaternary stereocenters

Seo Yeon Kim, Da Seul Lee[1], Eun Jin Cho[1,*]

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

Tertiary alkyl substrates have not been good substrates in enantioselective substitution processes because traditional S_N1 (unimolecular nucleophilic substitution) methods are not enantioselective, and the stereospecific S_N2 (bimolecular nucleophilic substitution) methods do not work for tertiary substrates. Therefore, development of new nucleophilic substitution processes of tertiary alkyl electrophiles, while providing stereospecific products under mild reaction conditions, would be highly desirable. Herein, we report a Ni-catalyzed stereospecific substitution process of easily available propargylic tertiary substrates for the construction of new C–C bonds. The ligand choice was critical for the efficiency and selectivity of the process.

Poster Presentation : **ORGN.P-462**

Organic Chemistry

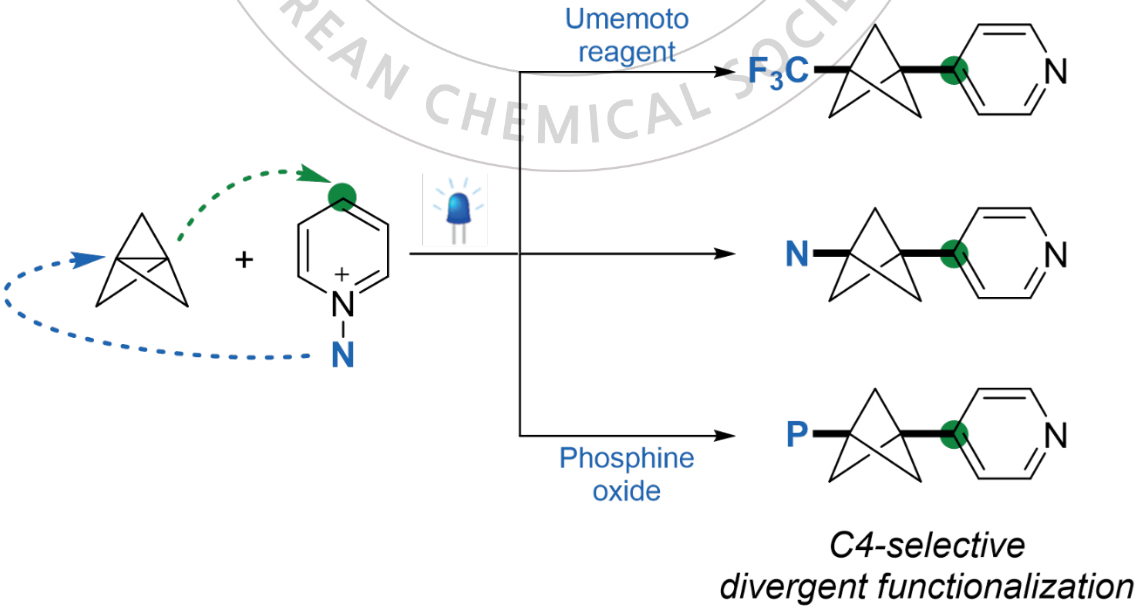
Exhibition Hall 1 FRI 11:00~12:30

Visible-Light-Induced 1,3-Difuntionalization of [1.1.1]Propellane: Pyridylation with N, P centered and CF$_3$ Radicals Using N-Aminopyridinium Salts

Wonjun Choi, Sungwoo Hong*

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

Strain-release pyridylation of [1.1.1]propellane was achieved using N-aminopyridinium salts. We could succeed direct installation of pyridyl group onto bicyclo[1.1.1]pentane (BCP) frameworks with three different functional groups(amidyl, phosphinoyl and trifluoromethyl groups) under visible-light irradiation. This method accommodates a broad scope and high functional group tolerance was demonstrated by late-stage modification of structurally complex biorelevant molecules. This protocol offers new approach to valuable pyridylated BCP motifs, which can be used bioisostere of some functional groups in drug discovery.



Poster Presentation : **ORGN.P-463**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

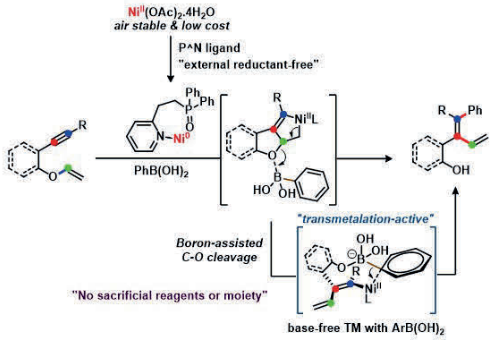
Syergistic Effects of Boron and Oxygen Interaction Enabling Nickel-Catalyzed Exogenous Base-Free Stereoselective Arylvinylation of Alkynes through Vinyl Transposition

Da Seul Lee, Hoimin Jung[1], Eun Jin Cho*

Department of Chemistry, Chung-Ang University, Korea

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

While organoboron compound is one of the most attractive and widely used nucleophiles in transition-metal-catalyzed coupling processes, they require sacrificial reagents for transmetalation (TM) processes. Herein, we report an unprecedented exogenous base-free procedure of a stereo-selective Ni-catalyzed arylvinylation of alkynes. It was revealed that Ni(0) species generated *in situ* from an air-stable Ni(II) precursor by a P^N ligand undergoes oxidative cyclization with an unactivated enyne to afford a nickellacycle intermediate, where a B-assisted C−O bond cleavage results in the formation of a TM-active boronate complex affording tetrasubstituted 1,3- diene products stereoselectively. A series of controlled experiments and density functional studies have been carried out to support the mechanistic proposal. The highly functionalized product comprising the stereoselective 1,3-diene system shows potential as an important building block in the synthesis of complex organic architectures.


Ni^II(OAc)2.4H2O
air stable & low cost
P^N ligand
"external reductant-free"
Ph
Ph
P
O
N
Ni^0
R
PhB(OH)2
O
Ni^IIL
B
HO
OH
R
Ph
OH
"transmetalation-active"
Boron-assisted
C-O cleavage
"No sacrificial reagents or moiety"
OH
OH
B
O
R
Ni^II
L
base-free TM with ArB(OH)2

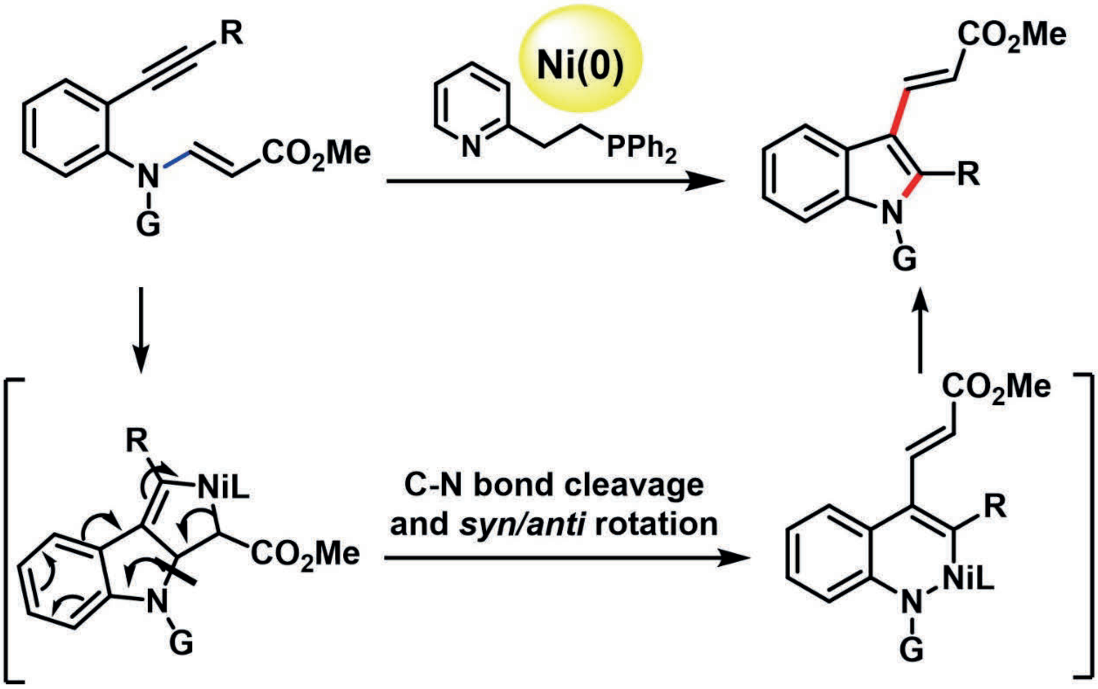
Poster Presentation : **ORGN.P-464**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Ni-Catalyzed trans-Carboamination across Internal Alkynes to Access Multi-Functionalized Indoles

Shrikant Tambe, Eun Jin Cho[1,*]

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

A Ni-catalyzed reaction was developed for the synthesis of multifunctionalized indoles. The reaction proceeded through oxidative cyclizationof the Ni(0)/P^N complex with an enyne system, 2-alkynyl anilinoacrylate, to provide a nickelacycle intermediate. The trans-carboamination around the internal alkyne was achieved by syn/anti-rotation of the Ni-carbenoid intermediate formed by C−N bond cleavage of the nickelacycle, and 3-alkenylated indoles were formed by C−N bond-forming reductive elimination. Notably, the synthesized indoles could be successfully transformed to functionalized carbazoles



√ Ni-catalysis √ ambient temperature √ alkenyl group migration
√ C-N bond cleavege and C-N/C-C bond formation

Poster Presentation : **ORGN.P-465**

Organic Chemistry

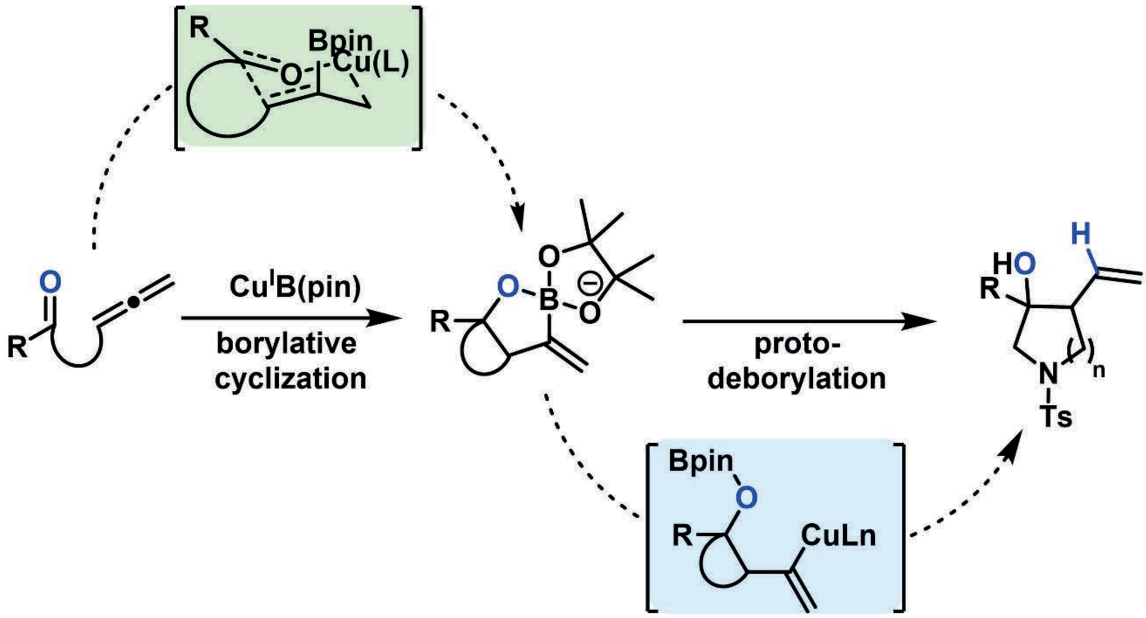
Exhibition Hall 1 FRI 11:00~12:30

Cu-Catalyzed Diastereoselective Reductive Cyclization of Allene-TetheredKetoamines

Ashraf Awais, Cheol Hyeon Ka[1], Shrikant Tambe[2], Eun Jin Cho[1,*]

Department of Chemistry, Chung-Ang University, Pakistan
[1]Department of Chemistry, Chung-Ang University, Korea
[2]Department of Chemistry, Chung-Ang University, India

A copper-catalyzed cascade process has been developed for the synthesis of 3-hydroxypyrrolidine derivatives in a highly diastereoselective manner. The reaction proceeded via borylative allyl copper intermediate formation from allenes; the intermediate underwent intramolecular diastereoselective cyclization, followed by cascade copper-catalyzed protodeborylation, to give 3-hydroxypyrrolidines. This method could be extended to the synthesis of 6-membered piperidine analogs. A series of control experiments were carried out to confirm the Cu-catalyzed facile protodeborylation of borylated homoallylic alcohols at room temperature.



Poster Presentation : **ORGN.P-466**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Carbamoyl Fluorides via a Selective Fluorinative Beckmann Fragmentation

Jinwoo Song, Hee Nam Lim[1,*]

Korea Research Institute of Chemical Technology, Korea
[1]*Department of Chemistry and Biochemistry, Yeungnam University, Korea*

We described a new synthetic method to afford carbamoyl fluorides. The design for the synthesis of carbamoyl fluorides is based on fluorinative Beckmann fragmentation of a-oximinoamides. During optimization, the Beckmann fragmentation appeared to be selective over competing Beckmann rearrangement. Diethylaminosulfur trifluoride (DAST) was a key reagent which activates the oxime and acts as fluoride donor. The substrates derived from secondary amines, lactams, and isatins were converted into the corresponding carbamoyl fluorides. Compared to other methods for preparation of carbamoyl fluorides, this protocol is fast and mild.

Poster Presentation : **ORGN.P-467**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

The effects of molecular weight and cross-linking density on hardness of PEG hydrogel

HyeonBi Jung, Se Won Bae*

Department of Chemistry, Jeju National University, Korea

Hydrogels, which have excellent biocompatibility and stability, are used as hygiene products such as contact lenses or absorbent layers for disposable diapers, and medical products such as capsules or dressings. Among these hydrogels, synthetic PEG hydrogels can be modularized by design, unlike natural hydrogels, to control functions or structural properties. However, the characterization of hydrogels in various environment such as buffer concentration, pH changes is not fully investigated. In this study, changes in stiffness, viscoelasticity, and swelling ratio of PEG hydrogels according to molecular weight of PEG backbone, concentration of buffer solution, and pH conditions were investigated. Various equivalents of multi-Arm PEGs were prepared and photopolymerized under UV light. Then, it was swollen in buffer solutions of various pH. Finally, the swelling ratio of hydrogels were measured with an electron microscope, and the stiffness and viscoelasticity of the hydrogel were measured with a rheometer.

Poster Presentation : **ORGN.P-468**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Total Syntheses of Iheyamines A and B via Cyanide-Catalyzed Imino-Stetter Reaction

Jiye Jeon, Jeongmin Jeon, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Iheyamines A and B were isolated from colonial ascidian polycitorilla sp. collected off the island of Iheya, Okinawa by Higa and co-workers in 1999. Unlike the fact that most of the nitrogen-containing polycyclic aromatic compounds isolated from ascidian are based on the pyrido[2,3,4-k,l]acridine moieties, these two natural products possess the unique azepino-2,2’-bisindole scaffold. In addition to their unique structural features, these alkaloids display cytotoxicity against several cancer cell lines. The unique structural features and intriguing biological activities of these alkaloids along with their very low bioavailability have prompted the chemical community to develop the total synthesis of these alkaloids. Despite their structural similarity, there have been no reports on the total synthesis of both iheyamines A and B even though two total syntheses of iheyamine A has been reported. Thus, the development of a more general synthetic route for the total synthesis of both alkaloids are highly desired.Very recently, our group developed novel method to construct unsymmetrical 2,2’-bisindole compound via the cyanide-catalyzed imino-Stetter reaction from 2-aminocinnamic acid derivative and indole-2-carboxaldehyde. Based on this protocol, we have started a program toward to the development of a synthetic route for Iheyamines A and B. 2-Aminocinnamic acid derivatives and N-protected-5-methoxyindole-2-carboxaldehyde gave the unsymmetrical 2,2’-bisindole compounds. Subsequent introduction of amino group at the 3’-position followed by intramolecular ring formation gave a lactam compound. From this intermediate, we were able to complete the total syntheses of both alkaloids. In this poster, the total syntheses of iheyamines A and B will be disclosed.

Poster Presentation : **ORGN.P-469**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Total Syntheses of 5,8’-Coupled Naphthylisoquinoline Alkaloids via Atroposelective Coupling Reaction Using an Internal Central Chirality

Young-In Jo, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Since naphthylisoquinoline alkaloids exhibit interesting biological activities and structural diversities, they have received considerable attention from the synthetic and medicinal communities. However, these natural products possess both central and axial chiralities, and thus they have been considered synthetically challenging targets. Even though a considerable number of methodologies to control central chirality have been reported, approaches to control the axial chirality have been far less developed. Furthermore, since most of the previous syntheses have utilized the isoquinoline moiety as a coupling partner, these approaches have been designed for the synthesis of a specific target molecule, and there were no general synthetic approaches to access these natural products.Recently, our group reported the asymmetric total syntheses of ancistrocladinium A, one of the N,C-coupled naphthylisoquinoline alkaloids, and its atropisomer via diastereoselective construction of axial chirality using the central chirality at the C3-position of the isoquinoline ring.1,2 As our continuing research towards the atroposelective syntheses of naphthylisoquinoline alkaloids, we investigated the atroposelective syntheses of C,C-coupled naphthylisoquinoline alkaloids using the internal central chirality in the isoquinoline ring. In this poster presentation, we will describe the asymmetric total syntheses of several 5,8’-coupled naphthylisoquinoline alkaloids via atroposelective Suzuki-Miyaura coupling reaction.3,4References1. Kim, K.-H.; Cheon, C.-H. Adv. Synth. Catal. 2016, 358, 2883.2. Kim, K.-H.; Cheon, C.-H. Org. Chem. Front. 2017, 4, 1341.3. Jo, Y.-I.; Lee, C.-Y.; Cheon, C.-H. Org. Lett. 2020, 22, 4653.4. Jo, Y.-I.; Lee, C.-Y. Cheon, C.-H. J. Org. Chem. 2020, 85, 12770.

Poster Presentation : **ORGN.P-470**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthetic Studies towards Yohimbine Alkaloids

Jihyun Kang, Eunjoon Park[1], Myunghoon Jeong[1], Cheol-Hong Cheon[1,*]

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

Yohimbine is one of the most well-known indole alkaloids with a rich chemical and medicinal history. The first total synthesis of the racemic compound was achieved more than 50 years ago by Van Tamelen and co-workers. Since the seminal synthesis, several other syntheses including asymmetric synthesis have been reported. Most previous syntheses of yohimbine commenced with a specific starting material containing the key fragment, , the ester group and the hydroxyl group at the C-16 and C-17 positions with appropriate stereochemistry, respectively. Subsequent construction of the C/D rings with tryptamine completed the synthesis of yohimbine. However, these conventional approaches required relatively lengthy synthetic sequences to control stereochemistry and to make pentacyclic structure.In this poster presentation, our endeavor towards the development of a new synthetic approach for yohimbine will be presented. The cyanide-catalyzed imino-Stetter reaction of aldimine derived from 2-aminocinnamic acid derivative and pyridine-2-carboxaldehyde bearing acetyl group at the C5-postionprovided the corresponding indole-3-acetic acid derivative. Subsequent formation of the 6-membered C-ring followed by Michael addition of the malonate at C-15 position provided a rapid access to the pentacyclic intermediate. By controlling the stereochemistry after next several steps, it is expected that synthesis of yohimbine alkaloids could be completed.

Poster Presentation : **ORGN.P-471**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Total Synthesis of Ngouniensine via Base-Catalyzed Indolization

Jinjae Park, Taewook Kim[1], Cheol-Hong Cheon*

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

Ngouniensine, isolated and structurally determined in 1982, is one of the major indole alkaloids of Strychnos ngouniensis. Unlike other indole monoterpene alkaloids, ngouniensine has unusual structural features. It possesses an exo-methylene group bridged to the C-2 position of the indole and the C-3 position of the secologanin. In addition, the two hydrogens at the C-3 and C-20 positions in the piperidine have a cis-relationship.The previous total syntheses of ngouniensine commenced with a starting material bearing the piperidine with the desired substituents and right stereochemistry. The indole subunit was introduced by the SN2 reaction of the piperidine compound with tryptophyl bromide. Subsequent intramolecular Friedel-Craft type reaction between indole C-2 position and carboxylic acid from the piperidine allowed thee seven-membered ring formation. The final introduction of the methylene group to ketone completed the synthesis of ngouniensine. However, this strategy generally required a rather lengthy sequence and control of the stereochemistry was often challenging.In this poster presentation, a novel strategy for the total synthesis of ngouniensine will be presented. Pyridine containing the substituents at the C-3 and C-20 positions was used as a surrogate for the key piperidine scaffold. Condensation of pyridine with 2-aminocinnamate followed by base-catalyzed indolization afforded the corresponding 2-(pyridylcarbonyl) indole-3-acetate. Subsequent reduction of acetate followed by activation of alcohol provided the tetracyclic scaffold containing the 7-membered ring and pyridinium ring. Syn-reduction of the pyridinium afforded the piperidine with right stereochemistry, and the introduction of the exo-methylene completed the total synthesis of ngouniensine.

Poster Presentation : **ORGN.P-472**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Atroposelective Total syntheses of 7,8’-Coupled Naphthylisoquinoline Alkaloids

Taelyn Kim, Young-In Jo, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Naphthylisoquinoline alkaloids have attracted considerable attention from the chemical community because of their unprecedented structural diversities and promising biological activities. However, because these natural products possess both central and axial chiralities, they have been considered synthetically challenging targets. Although 7,8’-coupled naphthylisoquinoline alkaloids consist of one of the main subclasses of these alkaloids, there have been very few total syntheses of the 7,8’-coupled naphthylisoquinoline alkaloids; only one example of the total synthesis of 7,8’-coupled naphthylisoquinoline alkaloid without no axial chirality was reported to date. Furthermore, no attempts to control atroposelectivity in the 7,8’-coupled naphthylisoquinoline alkaloids has been made so far. Recently, our group reported the total syntheses of naphthylisoquinoline alkaloids via atroposelective coupling reaction using the internal central chirality at the C-3 position of the isoquinoline ring as the atroposelectivity-controlling group.1,2 As our continuing efforts on the atroposelective total syntheses of naphthylisoquinoline alkaloids, we investigated the atropselective synthesis of 7,8'-coupled naphthylisoquinoline alkaloids using the internal central chirality in the isoquinoline ring as an atroposelectivity-controlling group. In this poster presentation, we will describe the asymmetric total syntheses of several 7,8'-coupled naphthylisoquinoline alkaloids.Reference1.Jo, Y.-I.; Lee, C.-Y.; Cheon, C.-H. Org. Lett. 2020, 22, 4653.2.Jo, Y.-I.; Lee, C.-Y.; Cheon, C.-H. J. Org. Chem. 2020, 85, 12770.3.Kim, K.-H.; Cheon, C.-H. Advanced Synthesis & Catalysis, 2016, 358, 2883-28884.Kim, K.-H.; Cheon, C.-H. Organic Chemistry Frontiers, 2017, 4, 1341-1349.

Poster Presentation : **ORGN.P-473**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Base-Catalyzed Synthesis of 2-(2-Nitroaryl)indole-3-Acetic Acid Derivatives

Juhyeon Park, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Since 2-aryl substituted indole-3-acetic acid derivatives exhibit biological activities, it is important to develop an protocol to access these scaffolds. Their biological activities depend on the substitution pattern in the indole moiety, particularly an electron-withdrawing substituent at the aryl moiety at the C2 position of the indole. Previously, our group has developed a new protocol to access theses building blocks by the cyanide-catalyzed imino-Stetter reaction of aldimines derived from 2-aminocinnamic acid and aryl aldehydes. Although the imino-Stetter reaction generally displays a broad substrate scope for both 2-aminocinnamic acid derivatives and aryl aldehydes, this protocol could not be applicable to aldimines derived from 2-nitrobenzaldehydes, leading to the indole products in low yield along with other side-products. To address the poor efficiency of the synthesis of 2-nitroaryl substituted indole-3-acetic acid derivatives via the cyanide-catalyzed imino-Stetter reaction, we developed a novel protocol to access 2-(2-nitroaryl)indole-3-acetic acid derivatives from N-(2-nitrobenzyl)-2-aminocinnamic acid derivatives via base-catalyzed cyclization followed by oxidation. Treatment of N-(2-nitrobenzyl)-2-aminocinnamic acid derivatives with a base afforded a benzylic anions, which underwent cyclization to the neighboring unsaturated ester, leading to 2-(2-nitroaryl)indoline-3-acetic acid derivatives. Subsequent oxidation of the indoline to the indole provided 2-(2-nitroaryl)indole-3-acetic acid derivatives by base-catalyzed synthesis strategy. In this poster presentation, we will disclose the base-catalyzed synthesis of 2-(2-nitroaryl)indole-3-acitic acid derivatives from N-(2-nitrobenzyl)-2-aminocinnamic acid derivatives via the base-catalyzed cyclization.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **ORGN.P-474**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

The characterization of the PEG hydrogels in various buffer solutions

Jiyun Kim, Se Won Bae[1,*]

Deparment of Chemistry, Jeju National University, Korea
[1]*Department of Chemistry, Jeju National University, Korea*

Hydrogels are widely used in fields such as tissue engineering and drug delivery based on their excellent biocompatibility and stability. Among them, PEG-based hydrogels can be easily prepared through convenient synthetic methods such as photo-polymerization. Furthermore, various functional groups can be easily introduced during the photo-polymerization step. These hydrogels show unique stiffness and viscoelasticity depending on the molecular weight of the PEG backbone and equivalents of the linker. In this study, the basic characteristics of these hydrogels were measured by the electron microscope and the rheometer, and their tendenciy of swelling ratios and stiffness according to the concentration and pH of the buffer solution were identified.

Poster Presentation : **ORGN.P-475**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Efficient Synthesis of Acetaminophen Using Continuous Flow Chemistry

Yoona Kang, Se Won Bae*

Department of Chemistry, Jeju National University, Korea

The demand for pain relievers such as acetaminophen is increasing due to the recent surge in the pandemic caused by the COVID-19. In particular, as the prescription of painkillers increases before and after vaccination, acetaminophen is not sufficiently supplied to the market in some countries. For these reasons, we used a continuous flow chemistry synthesis method rather than a conventional batch synthesis method to develop a safe and rapid mass production of acetaminophen. In this contribution, acetaminophen was successfully synthesized through the Beckmann rearrangement after the Vilsmeier reaction using nitroethane and polyphosphoric acid.

Poster Presentation : **ORGN.P-476**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Platinum-catalyzed ipso-Aryl Migration: Kinetic Evidence and Computational Analysis for the Occurrence of Diels-Alder Reaction

Alina Dzhaparova, Jin Kyoon Park*

Department of Chemistry, Pusan National University, Korea

The promising inter-and intramolecular cyclizations involving carbon-carbon triple bonds and nitrogen nucleophiles are regarded as powerful methods for the synthesis of substituted indoles. We have developed a novel methodology that employs PtCl4 and ortho-alkynyl-N-aryl sulfonamides substrates affording barrelene structure, which are key intermediate affording 2,3-disubstituted indoles through the Diels-Alder mechanism. The kinetic studies including primary 13C KIE and Hammett correlation revealed that the interdependence has coincided with the typical Diels-Alder reaction, which is as well supported with computational data. The operational simplicity, wide substrate scope, and high yields signify the prominent value of the present method for the synthesis of substituted indoles.

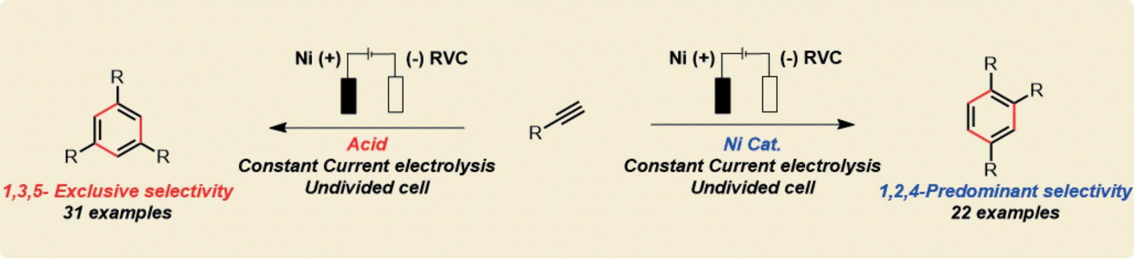
Poster Presentation : **ORGN.P-477**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Divergent Electrochemical [2+2+2] Cyclotrimerizations: Electron-mediated or Ni-catalyzed Cyclotrimerization?

Sagar Arepally, Jin Kyoon Park[1,*]

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

The development of green and sustainable synthetic methodologies to access structurally diverse organic compounds is a long-term aim for organic chemists. In this regard, electroorganic synthesis has been developed as an attractive catalytic platform, making use of renewable electricity instead of expensive conventionally used oxidants and reductants. Additionally, remarkable selectivity and reactivity can be observed in electrochemical conversions.All these aspects inspired us to involve in the development of novel electrochemical organic transformations. In this context, we described here, the regiodivergent electrochemical homo- cyclotrimerization of terminal alkynes to access trisubstituted benzene derivatives. Despite many conventional methods available for cyclotrimerization of terminal alkynes, the regioselectivity remains more challenging owing to the formation of a mixture of 1,2,4- and 1,3,5 regioisomers. To address this challenge, we attempted to take advantage of electrode materials, and the strategic choice of reagents and reaction conditions enabled an absolute regiodivergent cyclotrimerization of terminal alkynes. Furthermore, a plausible electroredox mechanism and radical pathway were proposed and supported by a series of electron paramagnetic resonance, radical clock experiments, cyclic voltammetry, and computational studies.



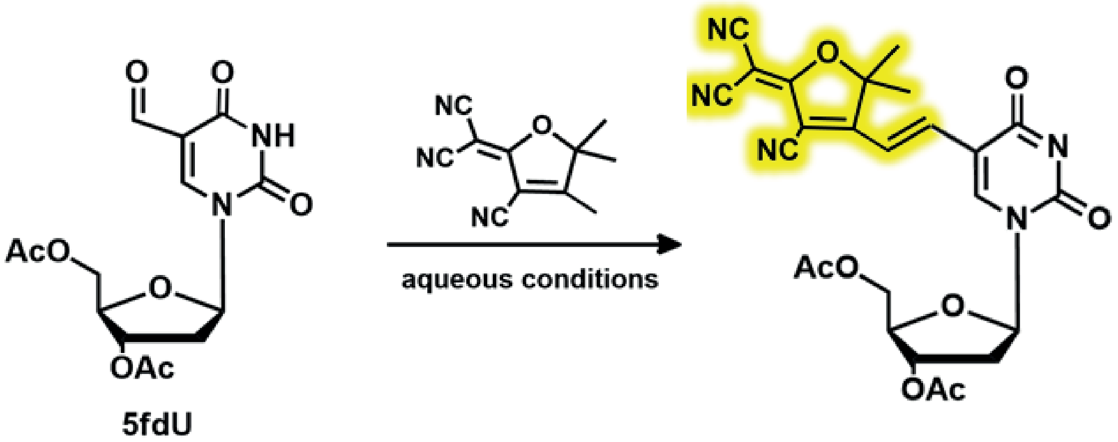
Poster Presentation : **ORGN.P-478**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

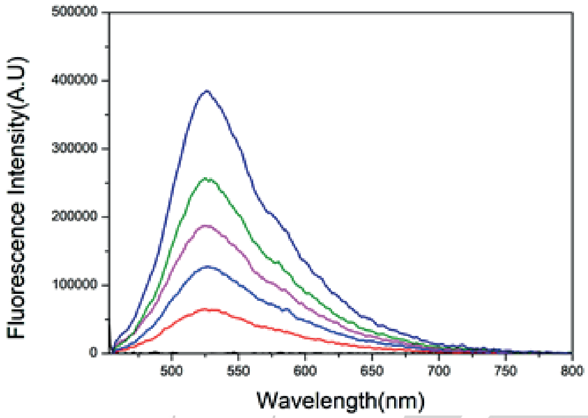
Design and synthesis of malononitrile-based fluorescent nucleosides and application to fluorogenic labeling of 5-formyluracil

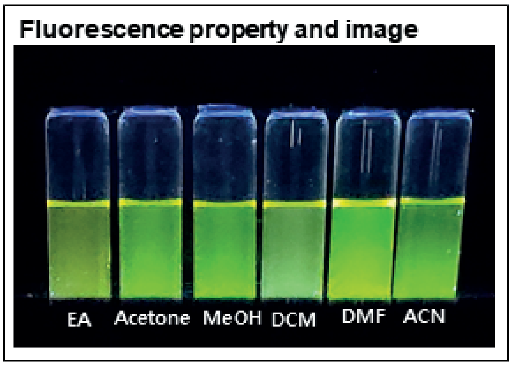
Hayeon Choi, Ki Tae Kim[*]

Department of Chemistry, Chungbuk Natioanl University, Korea

Fluorescent nucleosides have played essential roles in designs of functional nucleic acid systems for various biological applications (e.g. biosensors). In this context, developing novel fluorescent nucleosides featuring with new functionalities has become an important challenge. Herein, we report novel fluorescent nucleosides based on reactions of 5-formyluracil and malononitrile-based dye. The newly synthesized fluorescent nucleosides were readily synthesized under mild organic conditions as well as under aqueous conditions, showing high conversion rates and reaction yields. In addition, the synthesized fluorescent nucleosides were found to exhibit distinct yellowish green fluorescence attributed to a large stokes shift based on the push-pull type structure. Such advantageous features of the fluorescence nucleosides were finally applied to selective fluorescent labeling of 5-formyluracil, known as an important target in the epigenetics.






Fluorescence property and image

Poster Presentation : **ORGN.P-479**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Heterogeneous photocatalysis with graphitic carbon nitride for rearrangement of *N*-alkoxypyridinium salts

Minwoo Choi, Gyu-Yong Song*, Hyunjin Kim[1,*]

College of Pharmacy, Chungnam National University, Korea
[1]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*

Heterogeneous catalysts are recyclable catalyst which have attracted attention in chemical industries that can reduce waste and cost compare to transition metal catalysts. Graphitic carbon nitride (g-C_3N_4) is carbon based polymeric photocatalyst that could be active in visible light range, and it has physicochemical stability. A rearrangement of *N*-alkoxypyridinium salts for functionalization of pyridine was designed by graphitic carbon nitride catalyst in presence of visible light irradiation. The reaction was applied to access broad *N*-alkoxypyridinium substrate. The light dependency and reusability of catalysts was confirmed by light turn-on and off experiment, as well as recycling test.

Poster Presentation : **ORGN.P-480**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Photoinduced Pd-Catalyzed Formal Mizoroki–Heck Coupling of Unactivated Alkyl Chlorides

Geun Seok Lee, Soon Hyeok Hong*

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

The use of alkyl chlorides in Pd-catalyzed Mizoroki–Heck coupling reactions remains an unsolved problem despite its significant potential for synthetic utility and applicability. The combination of the high thermodynamic barrier of alkyl chloride activation and kinetic propensity of alkylpalladium complexes to undergo undesired β-hydride elimination has proved to be a significant challenge. Herein, a variety of alkyl chlorides, even tertiary chlorides, are shown to efficiently participate in Mizoroki–Heck cross-coupling reactions with excellent functional group compatibility under mild reaction conditions via photoinduced Pd catalysis. The reaction is applied to late-stage functionalizations of diverse biologically significant scaffolds and iterative double Mizoroki-Heck annulations, affording high molecular complexity in a single step. Notably, studies on the kinetic isotope effects in combination with DFT computations completely exclude the involvement of a previously proposed β-hydride elimination in the catalytic cycle, revealing that a chlorine atom transfer process is the key catalytic turnover step. This distinctive single-electron transfer mediated reaction pathway resolves a longstanding challenge in traditional two-electron-based Pd-catalyzed Mizoroki–Heck cross-coupling with alkyl electrophiles, wherein the β-hydride elimination is involved in the formation of both the desired product and undesired by-products.

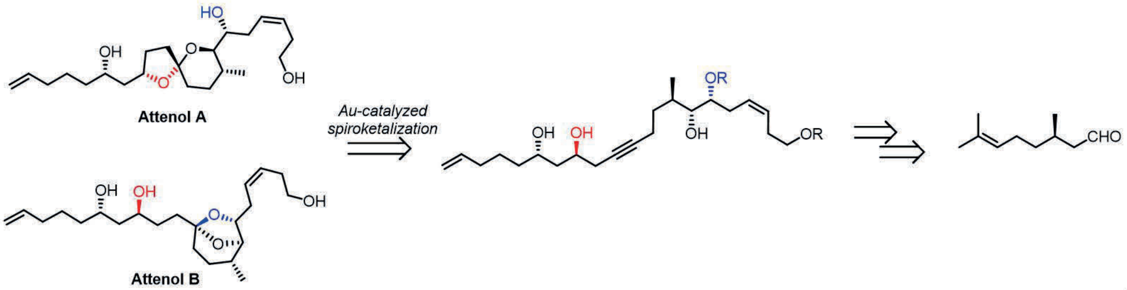
Poster Presentation : **ORGN.P-481**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Selective Total Syntheses of Attenols A and B via Gold catalyzed spiroketalization.

Ji Soo Shin, Hee-Yoon Lee[*]

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

Attenols A and B, isolates of Chinese bivale Pinna attenuate, are spiroketal isomers, which equilibrates in acidic conditions.[1] Attenol A is composed of a 5,6-spiroketal core, while Attenol B has unique 6,8-dioxabicyclo[3.2.1]octane (6,8-DOBCO), both having similarly functionalized side chains. Although several total syntheses of Attenols A and B were reported, synthetic approach to obtain the two isomers selectively from a common intermediate has not yet been established. We envisioned gold catalyzed spiroketalization of a common alkynyl-diol intermediate that can diverge into two pathways, resulting in the total syntheses of Attenols A and B selectively. References: (1) Takada, N.; Suenaga, K.; Yamada, K.; Zheng, S.-Z.; Chen, H.; Uemura, D. Chem. Lett. 1999, 1025-1026.



Poster Presentation : **ORGN.P-482**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Fluorescent sensor array based on Kaleidoscopic indolizine skeleton for glucose level monitoring in tears assisted by machine learning algorithm

Hyungi Kim, Eunha Kim[*]

Department of Molecular Science and Technology, Ajou University, Korea

It is still challenging to develop convenient yet precise monitoring system of glucose for improving glycemic control in person with diabetes. Most existing glucose monitoring systems have been developed as disposable strips using colorimetric, electrochemical and fluorescence penetrating skin for blood collection. These methods have limitations, such as accompanying pain for blood collection, increasing probability of viral infection depending on the examiner, and psychological stress for the patient. In order to overcome the limitations, more attractive approaches that measure blood glucose level non-invasively, such as skin patches, contact-lenses, and urine strips, have been conducted so far. Since, glucose in tears in a fasting state was measured as 0.1-0.3 mM in healthy people and 1-1.2 mM in diabetic patients, therefore, monitoring glucose level in tears have been spotlighted at promising method for monitoring blood glucose level in non-invasive manner. Here we develop a fluorescent array with a Kaleidolizine (KIz) system for accurate monitoring of glucose level in tears. To develop glucose-responsive fluorescent compounds for array composition, various boronic acids were introduced into the KIz core skeleton, allowing for the generation of 4 different fluorescent compounds. We confirmed that each fluorescent compound responded uniquely to hydrogen peroxide. Thus, by spotting compounds on cellulose paper along with glucose oxidase, which produce hydrogen peroxide via reaction with glucose, we generated 2 × 2 fluorescent sensor arrays for glucose monitoring. This small form-factor of the sensor array enables smartphone cameras to effectively capture fluorescence pattern changes of the array elements with respect to incubation with various concentration of glucose. Once images are captured, they are passed through several software components that extract the color differences from the sensor array image; a random forest-based machine learning model is then used to classify the expected glucose level of the sample that the sensor was exposed to. The sensor array consisting of a combination of 4 fluorescents derived a meaningful result of 99.3% (±0.2 step accuracy) through an HSV image machine learning algorithm-based analysis technique

according to the glucose concentration. Interest in convergence research between a sensor array made of fluorescence and machine learning is very attractive.

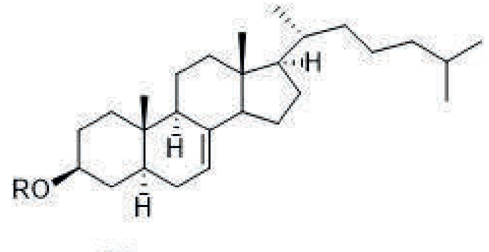
Poster Presentation : **ORGN.P-483**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and anti-inflammatory activity of $\Delta^{7(8)}$-5α-cholesten-3-ol and $\Delta^{7(8)}$-5β-cholesten-3-ol

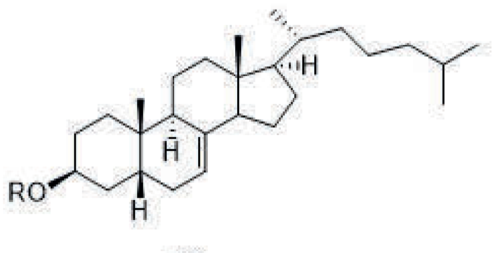
Dowon Yoon, Jung Woog Kim, Hakwon Kim[1,*]

Applied Chemistry, Kyung Hee University, Korea
[1] *Department of Applied Chemistry, Kyung Hee University, Korea*

Natural spinasterol-glucose (3-O-β-D-glucopyranosylspinasterol) isolated from Stewartia koreana leaves was identified as a potent anti-inflammatory compound. In our previous studies to find new sterols, it was found that the regioisomer of cholesterol, $\Delta^{7(8)}$-5-cholesten-3-ol (Lathosterol) and its derivatives exhibited the anti-inflammatory activity. In this study, to investigate the difference of anti-inflammatory activity between $\Delta^{7(8)}$-5α-cholesten-3-ol and its 5-anomer, $\Delta^{7(8)}$-5β-cholesten-3-ol, $\Delta^{7(8)}$-5α-cholesten-3-ol from 7-dehydrocholesterol and $\Delta^{7(8)}$-5β-cholesten-3-ol from chenodeoxycholic acid have been synthesized, respectively. Their anti-inflammatory activities have been investigated.



R=H, $\Delta^{7(8)}$-5α-cholesten-3-ol



R=H, $\Delta^{7(8)}$-5β-cholesten-3-ol

Poster Presentation : **ORGN.P-484**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Substrate-controlled chemo-/enantioselective synthesis of α-benzylated enals and chiral cyclopropane-fused 2-chromanone derivatives

Sunghyeon Ryu, Jung Woon Yang*

Department of Energy Science, Sungkyunkwan University, Korea

Catalytic, chemo-/enantioselective, and additional substrate-controlled processes via a cascade reaction are attractive challenges for synthetic organic chemists because structurally diverse molecule can be synthesized in a one-pot fashion via a single operation. In this regard, we were interested in developing substrate-controlled catalytic chemo-/enantioselective reactions using α,β-unsaturated carbonyl compounds, which are versatile building blocks for the synthesis of biologically active molecules and natural products. Substrate-controlled cascade reactions between α,β-unsaturated aldehydes or their analogues and 2,4-dinitrobenzyl chloride in the presence of a chiral secondary amine as the catalyst and base were developed, to obtain a broad spectrum of α-benzylated enals and enantioenriched cyclopropane-fused chroman-2-one derivatives. The cyclopropane-tethered iminium ion clearly served as a key intermediate in these reactions to trigger the formation of stereochemical outcomes, one of which was supported by a control experiment.

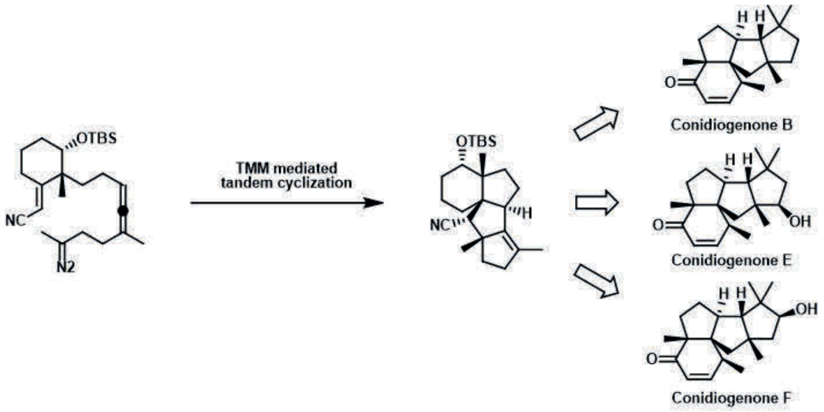
Poster Presentation : **ORGN.P-485**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Total synthesis of Conidiogenones

Hee-Yoon Lee*, Jiheon Kim

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

After first isolation of Conidigenone from fungus Penicillium cyclopium in 2002, more than 25 cyclopiane natural products has been isolated.[1] Conidiogenones possess 6-5-5-5 tetracarbocyclic structure with congested functional groups and thus became the subject of efforts toward the total synthesis by several research groups.[2] Herein, we would like to report a construction of 6-5-5-5 core structure of Conidiogenones via TMM mediated tandem cycloaddition reaction[3] and divergent total synthesis of natural products. The common intermediate from TMM cycloaddition was successfully executed to the total synthesis of Conidiogenone B, Conidiogenol, Conidiogenone E and Conidiogenone F. Reference1.Niu, S.; Fan, Z.-W.,; Xie, C.-L.; Liu, Q.; Luo, Z.-H.; Liu, G.; Yang, X.-W. *J. Nat. Prod.* **2017**, *80*, 2174‒2177.2.(a) Hou, S.-H.; Tu, Y.-Q.; Wang, S.-H.; Xi, C.-C.; Zhang, F.-M.; Wang, S.-H.; Li, Y.-T.; Liu, L., *Angew. Chem. Int. Ed.* **2016**, *55*, 4456‒4460. (b) Hu, P.; Chi, H. M.; DeBacker, K. C.; Gong, X.; Keim, J. H.; Hsu, I. T.; Snyder, S. A., *Nature.* **2019**, *569*, 703–707. (c) Xu B.; Xun W.; Su S.; Zhai H.; *Angew. Chem. Int. Ed.* **2020**, *59*, 16475–16479.3.(a) Kang, T.; Kim, W-Y.; Yoon, Y.; Kim, B. G.; Lee, H-Y.; *J. Am. Chem. Soc.* **2011**, *133*, 18050–18053. (b) Kang, T.; Song, S. B.; Kim, W-Y.; Kim, B. G.; Lee, H-Y.; *J. Am. Chem. Soc.* **2014**, *136*, 10274–10276. (c) Lee, H.; Kang, T.; Lee, H-Y.; *Angew. Chem. Int. Ed.* **2017**, *56*, 8254–8257.


OTBS
NC
N2
TMM mediated
tandem cyclization
OTBS
NC
H
H
H
O
Conidiogenone B
H
H
O
OH
Conidiogenone E
H
H
OH
O
Conidiogenone F

Poster Presentation : **ORGN.P-486**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Silaborative Assembly of Allenamides and Alkynes: Highly Regio- and Stereoselective Access to Trimetallic Skipped Dienes

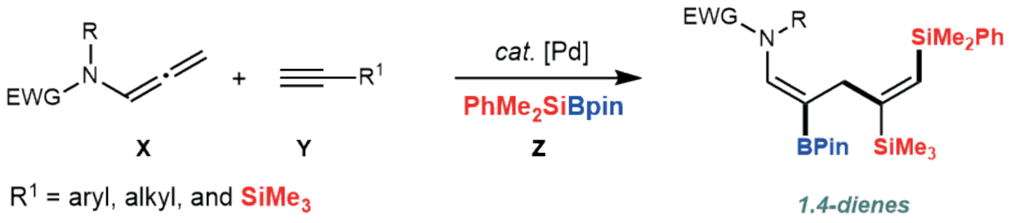
Tapas Ranjan Pradhan, Jin Kyoon Park[1,*]

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

During the past few years, our group has engaged in stereo- and regioselective functionalization through controlling the accessible intermediates from allenamides.1 Herein, we report the reaction discovery, generality, synthetic versatility, and computational mechanistic studies of a highly selective multicomponent reaction manifold to access 1,4-dienes bearing two chemically distinct C−[B] and C−[Si] bonds (Figure 1). Inspiration for the current research program arises from the facts that coupling strategies between two types of electronically-differentiated C−C π systems employing unsymmetrical interelement reagents (e.g. [Si]-[B]) remain unknown.2 To be sure, only intramolecular attempts have been reported employing predesigned enyne substrates, overall through two-component coupling approach.3 Thus, it is highly desirable to discover a multi-component atom-economy platform for such elusive goal. However, realization of this process via a multicomponent reaction employing a modularity-based silylboranes Z (e.g. Me2PhSi−Bpin) with allene (X) and alkyne (Y) has stood to be a formidable challenge for several interdependent reasons: (1) chemoselectivity, i.e. competitive interception of Z, [Si]−[B] reagent with either X4a or Y4b; (2) intrinsically feasible allene-alkyne coupling to form a regioisomer either XY1 or XY2 through hydroalkynylation1a; (3) competitive tandem pathways of allenamide either through a sequence of hydroalkynation/silaboration event or silaboration/alkyne interception pathways; and (4) typically challenging stereo- and regioselectivity issues known to be controlled by judicious choice of ligands or additive.

Our Atom Economy Proposal Toward tri-metallic Skipped Dienes

This work



[Highly stereo- and regioselective, Ligand-free condition, Late stage modifications]

Poster Presentation : **ORGN.P-487**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mitochondrial Targeting H_2S_n-Mediated Theranostic Agent for Inflammatory Disease

Ilwha Kim, Jungryun Kim, Yuvin Noh, Byungkook Kim, Saehee Rha, Zehra Zunbul, Minhyeok Choi, Youmi Choe, Jongseung Kim*

Department of Chemistry, Korea University, Korea

The insistent demand for space-controllable delivery, which reduces the side effects of non-steroidal anti-inflammatory drugs (NSAIDs), has led to the development of a new theranostics-based approach for anti-inflammatory therapy. The current anti-inflammatory treatments can be improved by designing a drug delivery system responsive to the inflammatory site biomarker, hydrogen polysulfide (H_2S_n). Here, we report a novel theranostic agent, consisting of three parts: H_2S_n-mediated triggering part, a two-photon fluorophore bearing mitochondria targeting unit (Rhodol-TPP), and anti-inflammatory COX inhibitor (indomethacin). In vitro experiments showed that theranostic agent selectively reacts with H_2S_n to concomitantly release both Rhodol-TPP and indomethacin. Confocal-microscopy imaging of inflammation-induced live cells suggested that theranostic agent is localized in the mitochondria where the H_2S_n is overexpressed. The theranostic agent reacted with H_2S_n in the endogenous and exogenous H_2S_n environments and in lipopolysaccharide treated inflammatory cells. Furthermore, theranostic agent suppressed both COX-2 level in the live cells and PGE2 level in blood serum, which are factors associated with inflammation-induced mouse models where H_2S_n is overexpressed. In vivo experiments with inflammation-induced mouse models suggested that theranostic agent exhibits inflammation-site-elective drug release followed by significant therapeutic effects, showing its function as a theranostic agent, capable of both anti-inflammatory therapy and precise diagnosis.

Poster Presentation : **ORGN.P-488**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

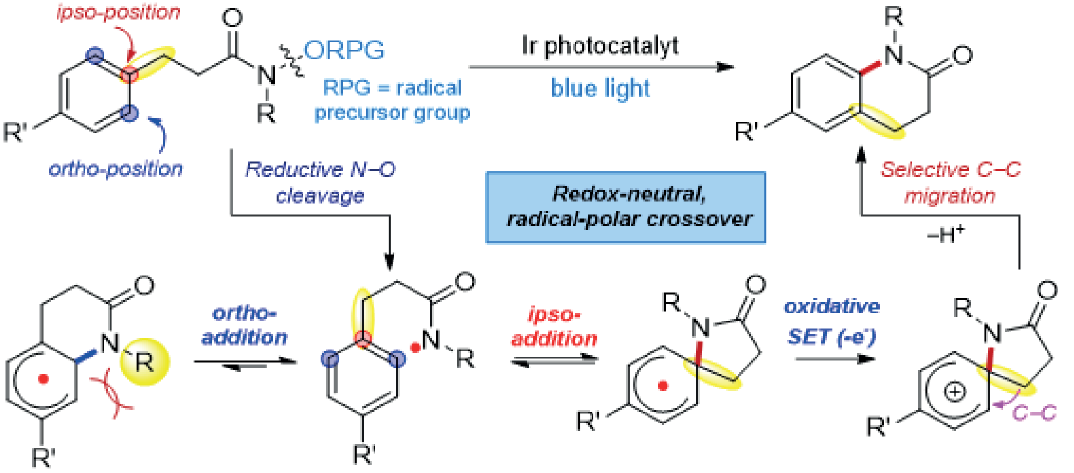
Visible-Light Induced C(sp^2)–H Amidation with an Aryl–Alkyl σ-Bond Relocation by Redox-Neutral Radical-Polar Crossover

Hyeyun Keum, Hoimin Jung, Jiwoo Jeong, Dongwook Kim[1], Sukbok Chang[*]

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

[1]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

We report an approach for the intramolecular C(sp^2)–H amidation of *N*-acyloxyamides under photoredox conditions to produce δ-benzolactams with an aryl–alkyl σ-bond relocation. Computational studies on the designed reductive single electron transfer strategy led us to identify *N*-[3,5-bis(trifluoromethyl)benzoyl] group as the most effective amidyl radical precursor. Upon the formation of an azaspirocyclic radical intermediate by the selective *ipso*-addition with outcompeting an *ortho*-attack, radical-polar crossover was then rationalized to lead to the rearomative ring-expansion with preferential C–C bond migration.



- *First example of visible-light induced selective radical ipso-addition and rearomative cyclization*
- *Conventional ortho-addition was blocked by steric tuning of the key amidyl radical intermediates*
- *Unique aryl–alkyl σ-bond relocation rationalized by radical-polar crossover of spirocyclic radicals*

Poster Presentation : **ORGN.P-489**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Radical Hydrodifluoromethylation of Alkenes via an Electroreductively Triggered Two-Pronged Approach

Seonyoung Kim, Hyunwoo Kim*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

The bioisosteric replacement of hydrogen atoms with fluorides has now become a standard requirement for new chemical entity to control biological properties such as metabolic stability, basicity, H-bond (HB) ability and bioavailability. Especially, the installation of difluoromethyl (CF2H) group into bio-relevent chemical structures has been an area of intensive research in drug development due to their unique ability in enabling effective lipophilicity and membrane permeability control. Despite their importance in pharmaceutical applications, synthetic routes to difluoromethylated pharmacophores are still very limited. To this end, we have devised a two-pronged strategy that enables hydrodifluoromethylation of a wide range of alkenes by means of reductive radical-polar crossover or direct hydrogen atom transfer from electroreductively generated carbon-centered radical intermediates. The newly developed strategy is generally valid to a wide range of alkenes and grant access to a late-stage modification of pharmacophores.

Poster Presentation : **ORGN.P-490**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

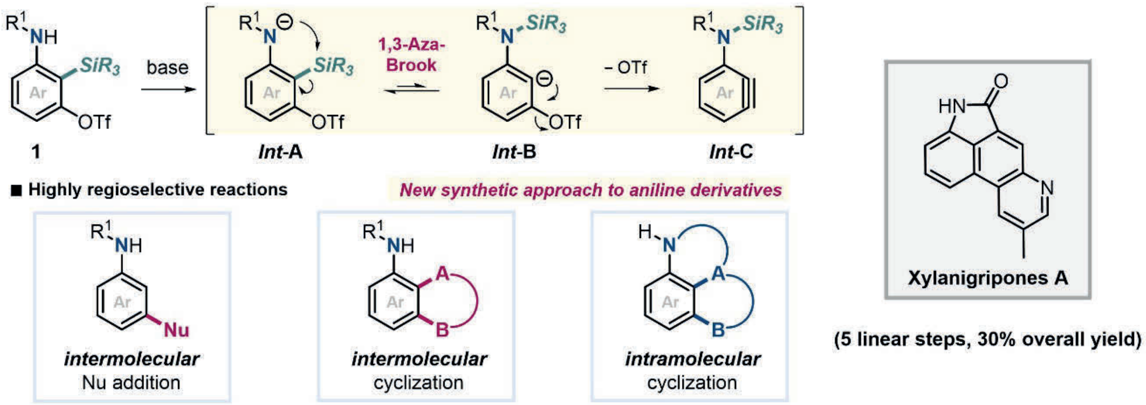
An 1,3-C-(sp2)-to-N silyl migration of aniline derivatives for the generation of 3-aminobenzyne intermediate

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

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

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

Design, synthesis, and validation of 3-amino-2-(trialkylsilyl)phenyl triflates have been achieved for the formation of highly reactive 3-aminobenzyne intermediate. 3-Aminobenzynes are potential intermediates with facile access to various aniline moieties embedded in bioactive compounds. The suggested base-activated aminobenzyne precursors effectively generate 3-aminobenzyne via C-(sp2)-to-N 1,3-aza Brook rearrangement, which are employed for the meta-selective nucleophilic additions, and inter- or intramolecular benzyne cycloadditions, allowing access to highly regioselective aniline derivatives.Through crossover experiment, the mode of anionic 1,3-silyl migration in this system was proved to be an intramolecular mechanism. For the amidobenzyne precursor, it is suggested that benzyne would be produced via a 1,5-Brook rearrangement. To gain insight into the regioselectivity observed in the reactions, density functional theory (DFT) calculations were performed. Finally, the method was applied as a key step for an ergot-type natural product, xylanigripones A, successfully synthesized from 3-amino-2-bromophenol in five steps with a 30% overall yield.



Poster Presentation : **ORGN.P-491**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

A highly selective fluorescent chemosensor using isothiocyanate functionality to detect H_2S

Jaekyong Kim, Doo OK Jang*

Department of Chemistry, Yonsei University, Korea

Hydrogen sulfide (H_2S) is one of the gaseous signaling molecules, related to important biological phenomena such as myocardial contraction and insulin secretion. Moreover, quantitative and qualitative analysis of hydrogen sulfide is significant because abnormal concentration of hydrogen sulfide is associated with diseases such as Down’s syndrome and liver cirrhosis. Therefore, developing sensors for sensing hydrogen sulfide is highly in demand.Herein, we designed a benzothiazole-based fluorescent chemosensor (named BT-ITC) having an isothiocyanate group. BT-ITC recognized hydrogen sulfide selectively over other biological analytes and metal ions in an aqueous solution. BT-ITC could detect hydrogen sulfide in 40 min. The detection limit was calculated to be 91 nM, showing its appropriative ability as a chemosensor for hydrogen sulfide at low concentration.

Poster Presentation : **ORGN.P-492**

Organic Chemistry

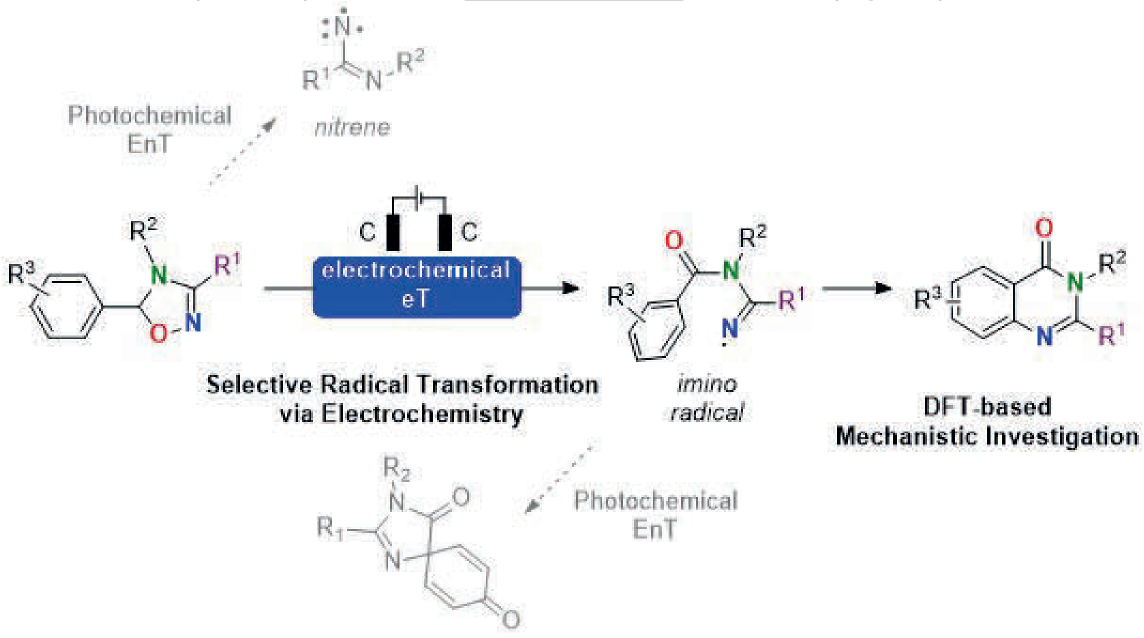
Exhibition Hall 1 FRI 11:00~12:30

Complementary Reactivity in Selective Radical Processes: Electrochemistry of Oxadiazolines to Quinazolinones

<u>Ho Seong Hwang</u>, Eun Jin Cho*

Department of Chemistry, Chung-Ang University, Korea

Electrochemistry has recently emerged as a sustainable approach to efficiently generate radical intermediates utilizing eco-friendly electric energy. An electrochemical process was developed to transform 1,2,4-oxadiazolines under mild conditions. The electrochemical N–O bond cleavage at a controlled oxidation potential led to the selective synthesis of quinazolinone derivatives that could not be obtained by photocatalytic radical processes, indicating complementary reactivities in radical processes. The electrochemical reaction pathways were fully revealed by DFT-based investigations.



Poster Presentation : **ORGN.P-493**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

α-L-fucosidase triggered cellular senescence imaging in vivo

Zehra Zunbul, Ilwha Kim[1], Yuvin Noh[1], Byungkook Kim[1], Jungryun Kim[1], Youmi Choe[1], Minhyeok Choi[1], Saehee Rha[1], Jongseung Kim[1,*]

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

Senescence is a stable state of irreversible cell-cycle arrest necessary for preventing the proliferation of damaged cells, promoting tissue remodeling, and maintaining organism homeostasis. The improper elimination of senescent cells can negatively affect the regenerative capabilities of tissues, thus contributing to local inflammation, age-related degenerative diseases, and cancer stemness and metastasis. However, there is still a need for convenient tools that can be used to probe the state of senescence and which allow the efficacy of senolytic drugs to be evaluated efficiently. Precise detection of cellular senescence may allow its role in biological systems to be evaluated more effectively, while supporting studies of therapeutic candidates designed to evade its detrimental effect on physical function. We report here studies of α-L-fucosidase (α-fuc) as a biomarker for cellular senescence and the development of an α-fuc-responsive aggregation induced emission (AIE) probe, probe designed to complement more conventional probes based on β-galactosidase (β-gal). Using this probe, the onset of replicative-, reactive oxygen species (ROS)-, ultraviolet A (UVA)-, and drug-induced senescence could be probed effectively. Probe also proved capable of identifying senescent cells lacking β-gal expression. The non-invasive real-time senescence tracking provided by this probe was validated in an in vivo senescence model. The results presented in this study lead us to suggest that probe could emerge as a useful tool for investigating senescence processes in biological systems.

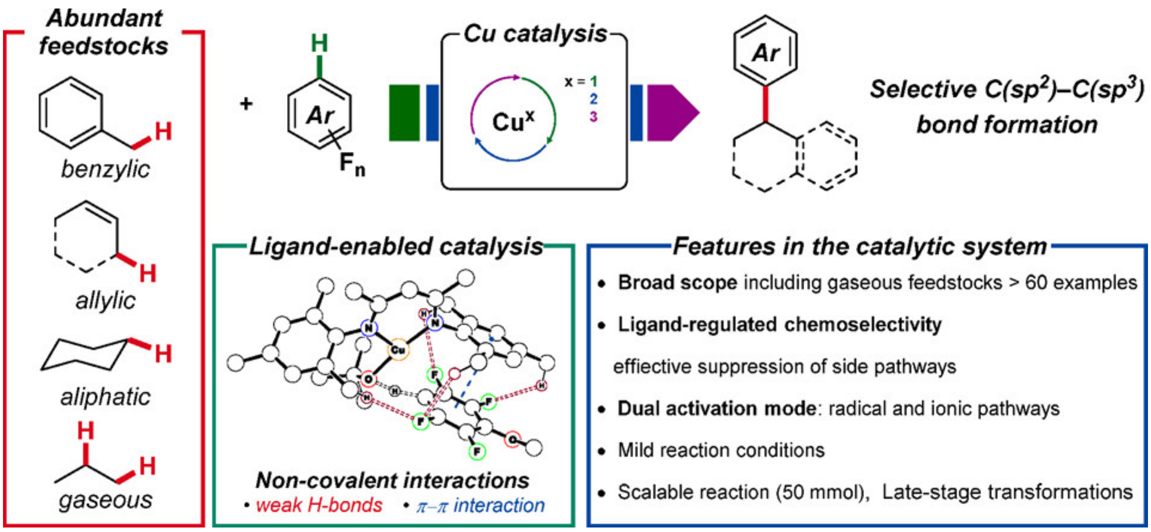
Poster Presentation : **ORGN.P-494**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Copper-Catalyzed Direct C–H Alkylation of Polyfluoroarenes by Using Hydrocarbons as an Alkylating Source

Weilong Xie, Joon Heo[1], Dongwook Kim[2], Sukbok Chang[1,*]

Chemical Engineering and Biotechnology, Donghua University, China
[1]Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[2]Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea

Construction of carbon–carbon bonds is one of the most important tools in chemical synthesis. In the previously established cross-coupling reactions, prefunctionalized starting materials were usually employed in the form of aryl or alkyl (pseudo)halides or their metalated derivatives. However, the direct use of arenes and alkanes via a 2-fold oxidative C–H bond activation strategy to access chemoselective $C(sp^2)$–$C(sp^3)$ cross-couplings is highly challenging due to the low reactivity of carbon–hydrogen (C–H) bonds and the difficulty in suppressing side reactions such as homocouplings. Herein, we present the new development of a copper-catalyzed cross-dehydrogenative coupling of polyfluoroarenes with alkanes under mild conditions. Relatively weak sp^3 C–H bonds at the benzylic or allylic positions, and nonactivated hydrocarbons could be alkylated by the newly developed catalyst system. A moderate-to-high site selectivity was observed among various C–H bonds present in hydrocarbon reactants, including gaseous feedstocks and complex molecules. Mechanistic information was obtained by performing combined experimental and computational studies to reveal that the copper catalyst plays a dual role in activating both alkane sp^3 C–H bonds and sp^2 polyfluoroarene C–H bonds. It was also suggested that the noncovalent π–π interaction and weak hydrogen bonds formed in situ between the optimal ligand and arene substrates are key to facilitating the current coupling reactions.



Features in the catalytic system

- **Broad scope** including gaseous feedstocks > 60 examples
- **Ligand-regulated chemoselectivity**
  effective suppression of side pathways
- **Dual activation mode**: radical and ionic pathways
- Mild reaction conditions
- Scalable reaction (50 mmol), Late-stage transformations

Poster Presentation : **ORGN.P-495**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Electrolytic C−H Oxygenation via Oxidatively Induced Reductive Elimination in Rh Catalysis

Seongho Jin, Jinwoo Kim[1], Dongwook Kim[1], Jung-Woo Park[1], Sukbok Chang[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, Korea*

Oxidatively induced reductive elimination has been considered as of high fundamental interest in transition metal catalysis for the reason that it facilitates kinetically challenging bond-forming process via alternative high-valent pathway, however its application toward efficient catalytic systems has been still less explored. In the current work, it was revealed that both anodic oxidation and chemical oxidation of a key rhodacyclic carboxylate intermediate enable the reductive elimination process to provide desired C–O bond construction even at room temperature. The accumulation of carboxylate anion near the anodic surface was rationalized to further induce the desired C–O bond-forming reductive elimination of Rh intermediate during electrolysis in particular. These findings guided us to develop Rh-catalyzed C–H oxygenation using stoichiometric amounts of readily accessible carboxylic acid coupling partners under mild electrolytic conditions. This synergistic approach demonstrates that electrolytic oxidation system offers new opportunity for developing mild and efficient catalytic method.

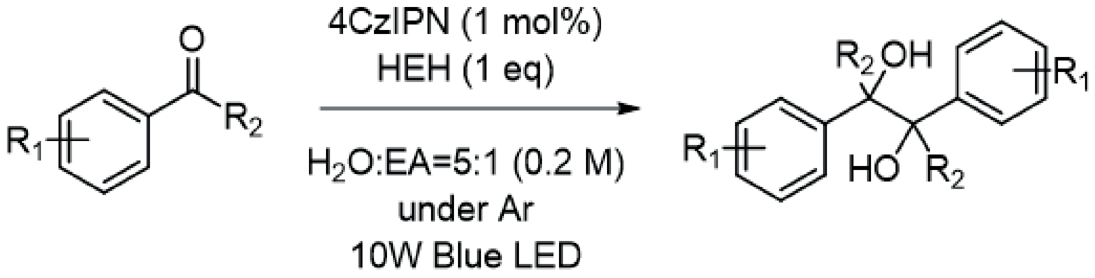
Poster Presentation : **ORGN.P-496**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Visible-light Photoredox Catalyzed Pinacol coupling in the Water

Hyunho Huh, Sang Kook Woo[1,*], Yejin Lee[2]

Organic chemistry, University of Ulsan, Korea
[1]*Department of Chemistry, University of Ulsan, Korea*
[2]*Chemistry, University of Ulsan, Korea*

The pinacol coupling is a powerful synthetic method for vicinally diols by carbon-carbon bond formation. Basically, traditional pinacol coupling reaction use stoichiometric amount of metal reductants (Mg, Al, Zn, Mn, etc.). However, these methods can cause environmental issues. To resolve this problem, we decide to use the organic photocatalyst as a reductant instead of metal reductants. Although photoredox catalyzed pinacol coupling reactions have been developed, many methods use expensive transition metals as a photocatalysts. These methods still have an economical and environmental problem. We consider the 4CzIPN as an organic photocatalyst which is inexpensive and easy to prepare. It is also greener and economical by using water as a solvent. The developed method shows excellent functional group tolerance with a broad substrate scope and good to excellent yield.



Poster Presentation : **ORGN.P-497**

Organic Chemistry

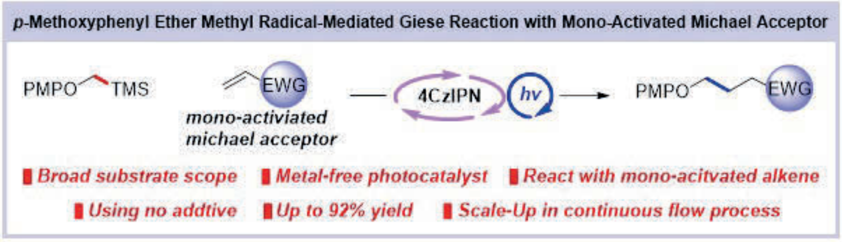
Exhibition Hall 1 FRI 11:00~12:30

Photoredox-Catalyzed Hydroalkoxymethylation of Various Michael acceptors and Alkoxymethyl Radicals

Ran Hui Kim, Sang Kook Woo*

Department of Chemistry, University of Ulsan, Korea

We report a photoredox-catalyzed hydroalkoxymethylation of various Michael acceptors with alkoxymethyl radicals. The Giese reaction of a variety of mono-activated Michael acceptors with alkoxymethyl radical intermediates which are generated by single electron oxidation of alkoxymethyltrimethylsilane using 1,2,3,5-tetrakis(carbazole-9-yl)-4,6-dicyanobenzene (4CzIPN) as photocatalyst The developed method shows excellent functional group tolerance with a broad substrate scope and good to excellent yield. Furthermore, the developed protocol is applicable in continuous flow process with short reaction times for the scale-up.



Poster Presentation : **ORGN.P-498**

Organic Chemistry

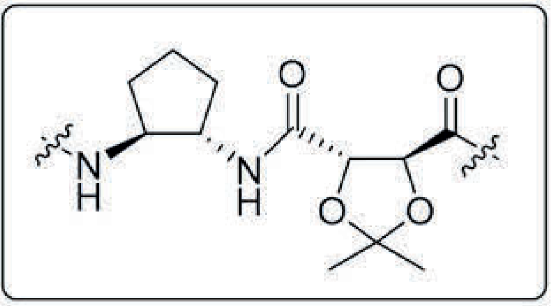
Exhibition Hall 1 FRI 11:00~12:30

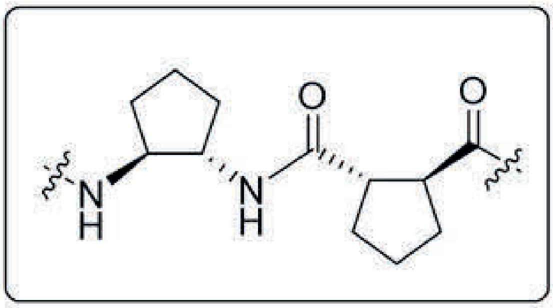
Helical structures of nylon-like oligomers containing 1,2-diamine and 1,2-dicarboxylic acid residues with a five-membered ring constraint

Soo Hyuk Choi*, Sunglim Choi

Department of Chemistry, Yonsei University, Korea

A series of nylon-like oligomers were synthesized by the alternation of cyclic 1,2-diamine and 1,2-dicarboxylic acid building blocks with a five-membered ring constraint. The nylon 2 4 oligomers are symmetric and display helical structures that are similar to the β-peptide 12-helix with intramolecular 12-atom ring hydrogen bonds. The cyclopentane moiety sufficiently preorganize each building block to promote 12-helical folding. In addition, the acetonide derivative of tartaric acid increase the solubility of the oligomers and promote helical folding.


N
H
N
H
O
O
O
O


N
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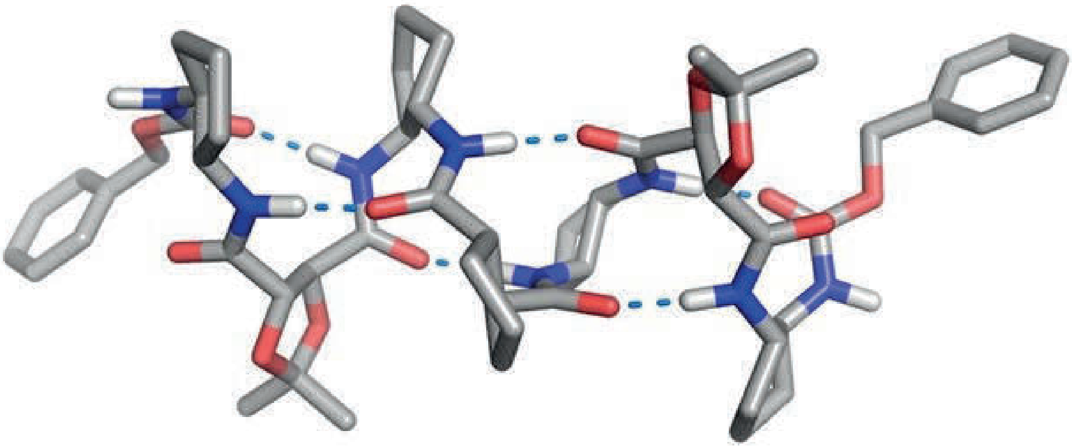


Poster Presentation : **ORGN.P-499**

Organic Chemistry

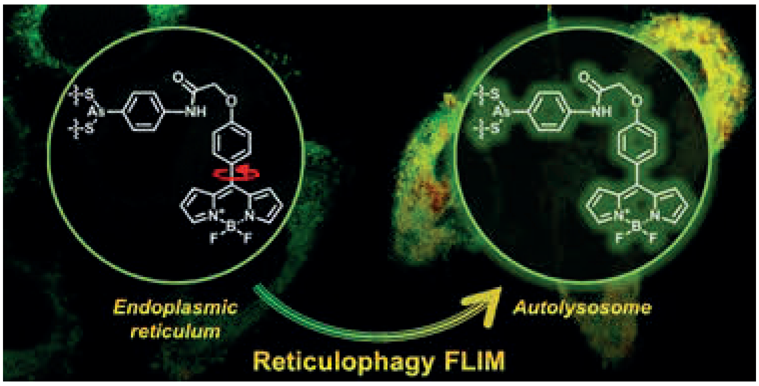
Exhibition Hall 1 FRI 11:00~12:30

A Novel Bifunctional Turn-ON Fluorogenic Molecular Rotor for Lifetime Imaging of the Endoplasmic Reticulum Microviscosity during Reticulophagy

Yuvin Noh, Ilwha Kim, Jungryun Kim, Youmi Choe, Saehee Rha, Byungkook Kim, Minhyeok Choi, Zehra Zunbul, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Autophagy of the endoplasmic reticulum (ER) is selective autophagy associated with the unfolded protein response for maintaining cell homeostasis, termed reticulophagy or ER-phagy. Protein quality control pathways in the ER are mainly contributed to the ER-phagy. Nevertheless, ER stress can result in several diseases such as tumorigenesis, neurodegenerative diseases, and diabetes. Thus, a broad understanding of the reticulophagy process could provide a potential advent of new technology for the diagnosis and therapy of these diseases. Herein, we report a novel bifunctional fluorescent molecular rotor, which image ER microviscosity during reticulophagy. This dual-functional and microenvironment-sensitive fluorescent probe was rationally designed to covalently bind to vicinal dithiol-containing proteins (VDPs) in the ER. Therefore, the selective binding of VDPs in the ER leads to reticulophagy initiation and microviscosity evaluation. Furthermore, the molecular rotation of the probe allows us to explore the dynamic changes of the microenvironment in sub-organelles during the formation of autolysosome. Consequently, the novel fluorogenic probe could be adopted as a promising diagnostic for the study of ER autophagy.



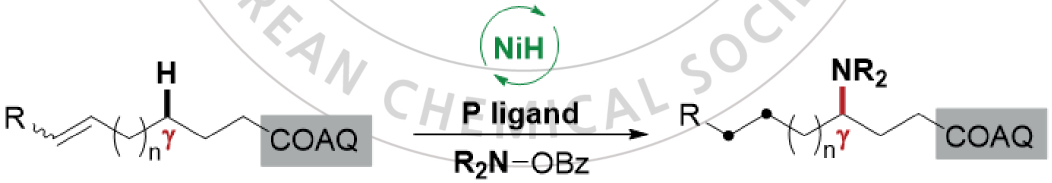
Poster Presentation : **ORGN.P-500**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

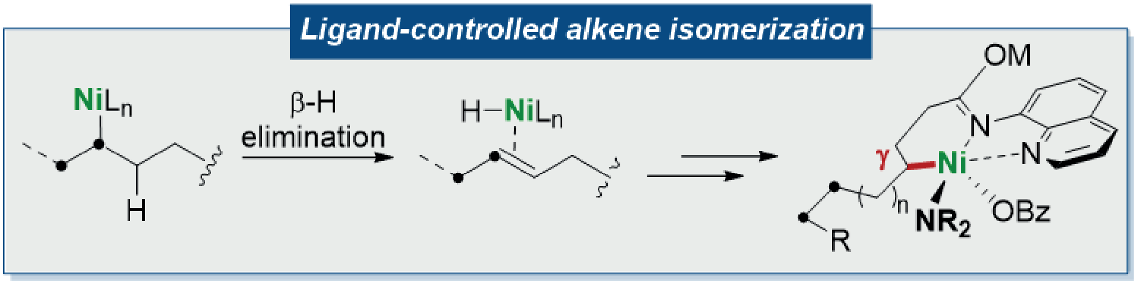
NiH-Catalyzed Alkene Isomerization-Hydroamination: A Strategy for Remote C(sp^3)–H Amination with γ-Selectivity

Huiyeong Seo, Sungwoo Hong[*]

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

Remote olefin functionalization has continuously attracted much attention in chemical synthesis, which can install functionalities at inert sp^3 C–H sites. However, this alkene isomerization/functionalization process has been restricted to C(sp^3)–H bonds α or β to polar-characteristic units, while the access to γ- or more remote sites via controlled alkene transposition has not been developed yet. Herein, we represent γ-selective migratory hydroamination through NiH catalyzed alkene isomerization by external ligand and thermodynamically stable 8-aminoquinoline (AQ)-chelated nickellacyle, subsequently interrupted by an aminating reagent. Furthermore, unprecedented δ-selective amination was achieved by picolinamide (PA)-coupled alkene substrates to extend the synthetic utility of this protocol.





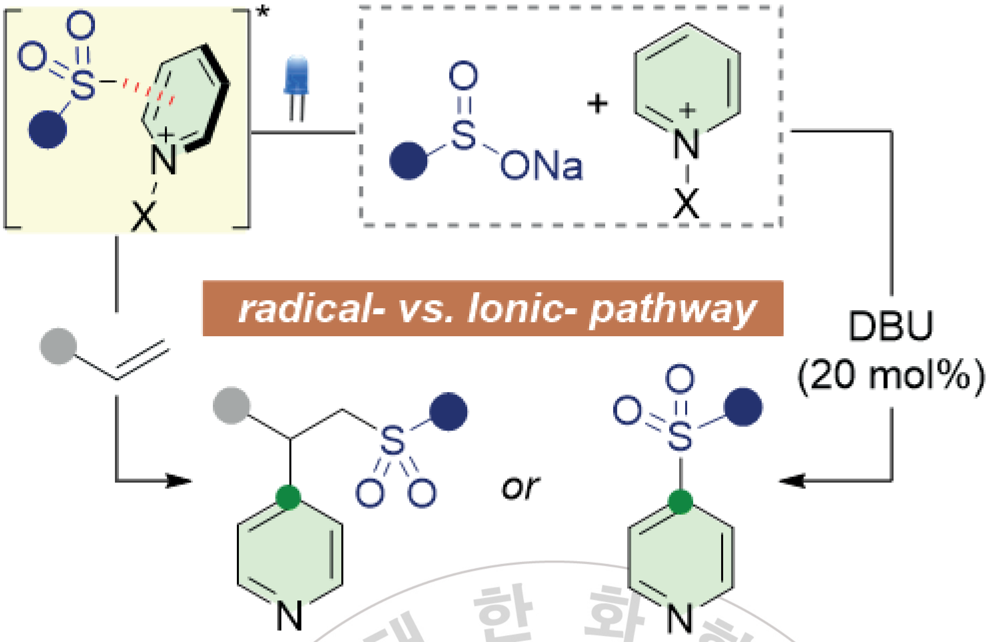
Poster Presentation : **ORGN.P-501**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Divergent Synthetic Approach of Sulfinates with Pyridinium Salts Based on Radical versus IonicPathways

Euna You, Sungwoo Hong*

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

One of the main objects for the efficient synthesis of diverse compounds in modern organic chemistry is to develop reaction pathways that are distinguished from identical starting materials. We discovered a combination of pyridinium salts and sulfinates to achieve the sulfonative pyridylation of alkenes and direct C4-sulfonylation of pyridines by controlling the radial versus ionic pathway for selective formation of each product. As using a base, sulfonyl groups can be directly incorporated to the C4 position of pyridines. Notably, the reactivity of this set of compounds is completely changed upon visible-light irradiation: electron donor-acceptor (EDA) complexes of *N*-amidopyridinium salts and sulfinates provide access to sulfonyl radicals. In this catalyst-free radical pathway, both sulfonyl and pyridyl groups could be installed into alkenes through a three-component reaction, which provides facile access to a variety of β-pyridyl alkyl sulfones. These two reactions are orthogonal and complementary and a broad substrate scope in a late-stage functionalization under mild conditions is also achieved.



- divergent reactivity by activation mode
- excellent functional group tolerance
- photocatalyst-, oxidant-free
- C4-selective pyridylation

Poster Presentation : **ORGN.P-502**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

MDM2-Related Cellular Apoptosis Provoked by Clusterization-Triggered Emission Spiropolymer Therapeutics

Youmi Choe, Zehra Zunbul, Minhyeok Choi, Byungkook Kim, Yuvin Noh, Ilwha Kim, Jungryun Kim, Saehee Rha, Jongseung Kim*

Department of Chemistry, Korea University, Korea

We successfully synthesized spiropolymers containing heteroatom by adopting multicomponent spiropolymerization (MCSP), an efficient synthetic tool for building spiropolymers without catalysts. Strong interaction between P1a2b, one of the most potent spiropolymers, leads to cluster-triggered emission (CTE). Blocking the anti-apoptotic p53/MDM2 interaction results in P1a2b-induced cancerous cellular apoptosis. Various studies, including solution and cell-based experiments, demonstrate that these spiropolymers have good biocompatibility while non-toxic in normal cells. Additional studies (e.g., computational docking studies, cellular cytotoxicity assay, and protein expression experiments) suggest the spiropolymers as a potent fluorescent diagnostic and an effective therapeutics for cancer.

Poster Presentation : **ORGN.P-503**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

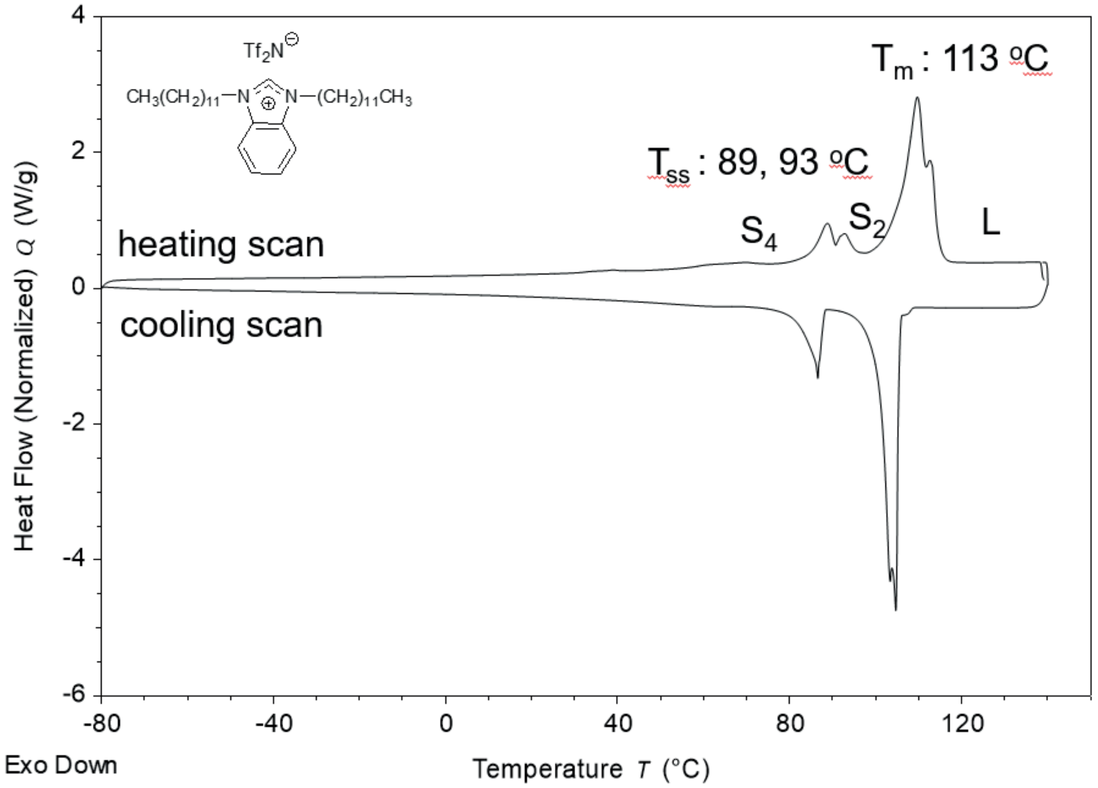
Synthesis and characterizations benzimidazolium salts and their thermal properties

Seunghwan Kim, Minjae Lee[1,*]

Kunsan National University, Korea

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

Organic ionic plastic crystals (OIPCs) are soft crystalline solid and they can be applied to solid-state electrolytes. Many types of organic cation salts have been applied, however material spectrum for the electrolytes of Li-ion batteries is very narrow. By our research group, various structures of ammonium based organic cations were reported. In this study, a series of 1,3-dialkylbenzimidazolium salts coupled to Br^-, PF_6^-, Tf_2N^- and BF_4^- anions with different linear alkyl chain lengths are synthesized as a new type of OIPCs. 1,3-Dialkylbenzimidazolium salts with Tf_2N^- anions show highest thermal stability from thermal gravimetric analysis. Using differential scanning calorimetry (DSC), we find that 1,3-diethylbenzimidazolium Br^- exhibits multiple solid-solid phase transitions (T_{ss} = 26, 112, 161 ℃) below its melting temperature. Also, 1,3-diethylbenzimidazolium Br^- shows low entropy of fusion, 10 J $K^{-1}mol^{-1}$, which satisfies the Timmerman' definition of plastic crystals ($\Delta S_f < 20$ J $K^{-1}mol^{-1}$).


$Tf_2N^{\ominus}$
$CH_3(CH_2)_{11}$—N—$(CH_2)_{11}CH_3$
T_m : 113 ºC
T_{ss} : 89, 93 ºC
S_4
S_2
L
heating scan
cooling scan
Heat Flow (Normalized) Q (W/g)
4
2
0
-2
-4
-6
-80
-40
0
40
80
120
Exo Down
Temperature T (°C)

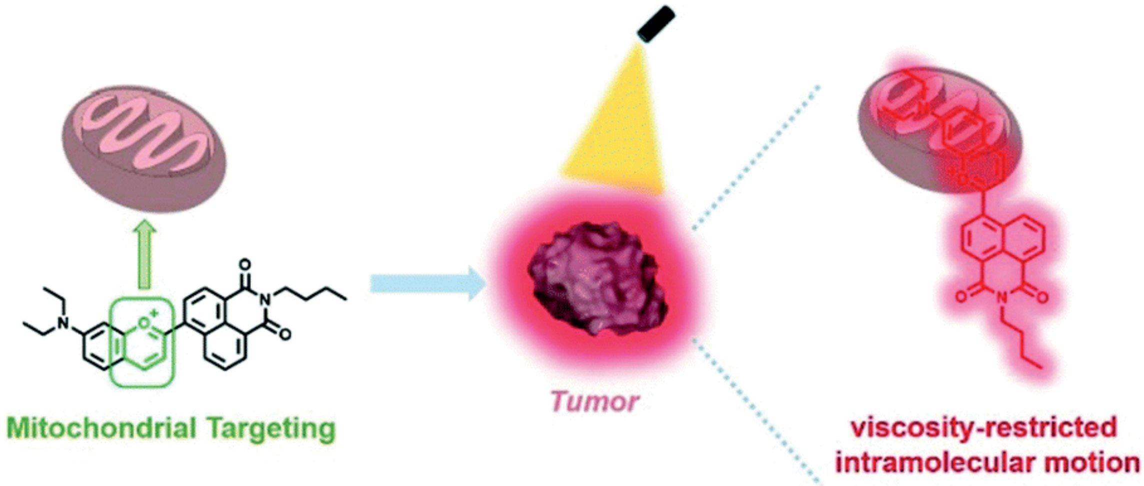
Poster Presentation : **ORGN.P-504**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Selective tumor imaging by combining viscosity-restricted intramolecularmotion and mitochondrial targeting

<u>Jungryun Kim</u>, Ilwha Kim, Yuvin Noh, Saehee Rha, Minhyeok Choi, Byungkook Kim, Zehra Zunbul, Youmi Choe, Jongseung Kim*

Department of Chemistry, Korea University, Korea

We report here a novel fluorescent molecular conjugate, V-M1, enabling an accurate visualization of tumor tissues. V-M1 has an emission wavelength of over 650 nm, which is well within the therapeutic near-infrared range. Near-infrared fluorescence covering the first therapeutic window (650–900 nm), where absorbance, light scattering, and autofluorescence are low, can be used to achieve tissue selectivity and orthogonality of fluorescence with tissue autofluorescence. This cationic dye accumulates in tumors, allowing malignant cells to be visualized as a function of mitochondrial viscosity. Moreover, this positive charge provides mitochondrial selectivity towards the molecular conjugate and significantly makes the higher mitochondrial potential of cancerous tissues. This probe not only avoids possible concerns with cell membrane viscosity but also boosts the selectivity towards malignant tissues when compared to other viscosity probes.



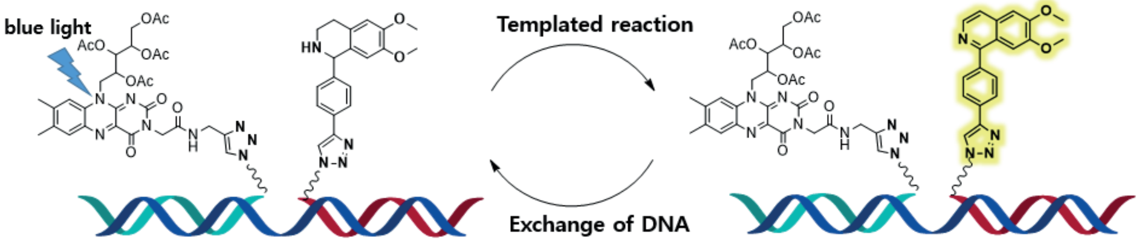
Poster Presentation : **ORGN.P-505**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Riboflavin-Catalyzed Fluorogenic Photooxidation for Nucleic Acid Sensing

Hokyung Kim, Ki Tae Kim[1,*]

Chemistry, Chungbuk Natioanl University, Korea
[1]*Department of Chemistry, Chungbuk Natioanl University, Korea*

Nucleic acid-templated reactions proceed by high effective concentrations induced by hybridization of reactive oligonucleotides to a template sequence. One of the promising features of nucleic acid-templated reactions is signal amplification arising from iterative cycles of strand exchange and chemical reactions. Such an advantageous feature enables the design of amplification-based nucleic acid-sensing platforms that release or synthesize fluorescent molecules only in the presence of target nucleic acids. Although template reactions are currently being considered a powerful technique for nucleic acid-sensing, however, they suffer from low signal amplification. Therefore, improvements are still needed and this can be achieved by expanding the chemical scope of template reactions. Here, we report novel nucleic acid-templated reactions based on riboflavin-catalyzed fluorogenic oxidation of a cyclic amine. The cyclic amine is oxidized by riboflavin under blue-light irradiation to produce a fluorescent isoquinoline moiety. Using these new simple photoreactions, we can effectively detect specific target nucleic acids with bright fluorescence signals.



Poster Presentation : **ORGN.P-506**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Acidochromic and Photochromic Reaction of Some Spiropyran-sulfonate Derivatives

Go Eun Choi, Eun Ju Shin[*]

Department of Chemistry, Sunchon National University, Korea

Spiropyran is a well-known photochromic compound. Under the irradiation of UV light or with the addition of metal cation, ring-closed spiropyran converts into the ring-opening merocyanine. On the addition of an acid, it undergoes ring opening to form protonated merocyanine. With the addition of a base, protonated merocyanine reverts into the ring-closed spiropyran. Because spiropyran derivatives are easy to synthesize and exhibit a distinct color change due to reversible structural transformation, and high fatigue resistance, various excellent sensors based on spiropyran have been developed for metal cation detection and pH measurements.Irreversible photoacids releasing a strong acid upon photolysis are mainly used as initiators and resists. Reversible photoacids that exhibit stronger acidity in the excited state than in the ground state show the disappearance of the proton accumulation when light irradiation is switched-off. In order to accumulate large amount of protons under low power continuous irradiation and despite very short lifetimes (1~100 ns), their proton release must be coupled with a slow isomerization process.In polar acidic medium, sulfonate-functionalized protonated merocyanine MEH-SO3-(Φr=0.37 in DMSO, pKa=7.8) behaves like long-lived reversible photoacids and attracts great interest for the pH-responsive light-controlled proton transfer reaction.In this study, reversible acidochromic and photochromic reaction of spiropyran-sulfonate derivatives has been investigated at various pH and UV or visible light on/off conditions using absorption and fluorescence spectroscopy.

Poster Presentation : **ORGN.P-507**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Unsymmetrical 3,5-Disubstituted-2-Pyridones via Protecting Group-Controlled Regioselective Functionalization in Batch and Flow Chemistry

Yong-Ju Kwon, Won-SuK Kim[1,*]

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

2-Pyridones, six-membered N-heterocycles containing amide group, are an important skeletal motif found in a number of natural products and pharmaceutical drugs. In particular, unsymmetrical 3,5-disubstituted-2-pyridones are serve as a valuable synthon in drug molecules, such as amrinone and milrinone (phosphodiesterase enzyme inhibitors), prescribed intravenously for congestive heart failure. Preferentially, we screened the protecting group on 3,5-dibromo-2-hydroxypyridine for different steric or electronic environment of two bromines. Along with the employment of different protecting groups, di-tert-butylisobutylsilyl (BIBS) and toluene sulfonyl (Ts) groups, the various functionalization on C3 and C5 of the synthesized starting material proceeded in a highly regioselective manner and further elimination reaction furnished 2-pyridones derivatives in good to excellent yields. In addition, one-pot synthesis and further investigation, C–N, C–CN and C–Si bond formation reactions, were conducted to demonstrate the practical convenience of the strategy. Finally, amrinone and milrinone, cardiotonic drugs were successfully synthesized in total three steps from 3,5-dibromo-2-hydroxypyridine with 41% and 56% overall yields.

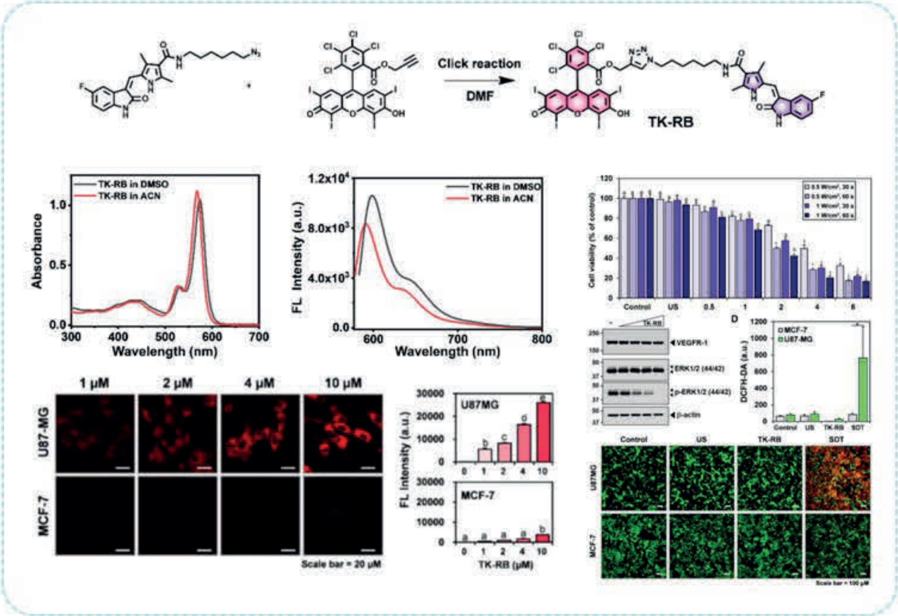
Poster Presentation : **ORGN.P-508**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Targeting VEGFR associated glioblastoma tumor models using ultrasound activatable anti-angiogenic sonosensitizer

Saehee Rha, Youmi Choe, Ilwha Kim, Jungryun Kim, Yuvin Noh, Byungkook Kim, Minhyeok Choi, Zehra Zunbul, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Angiogenic signaling pathway is a crucial contributing factor in tumor recurrence and development, which can induce substantially diminished treatment outcomes, particularly in the oxygen-dependent photo and sonodynamic therapies. VEGF (Vascular Endothelial Growth Factor) play a vital role in angiogenesis progression : precisely, upregulated VEGF signaling is closely linked with angiogenesis progression in many types of cancers. Here in, we present a sunitinib-conjugated sonosensitizer (TK-RB : Tyrosine Kinase-Rose Bengal) to strengthen the anti-cancer efficacy via VEGF inhibition-mediated anti-angiogenesis along with cellular/tumor damage by ROS(Reactive Oxygen Species) generated under ultrasound irradiation. TK-RB reveals superb selectivity and cytotoxicity toward VEGF-(+) cells (U87MG) over VEGFR-(-) cells (MCF-7). The fluorescent imaging analysis in vivo/ex vivo and the tumor growth examination in nude mice with U97MG glioblastoma tumor xenografts demonstrate that TK-RB provides an improved anti-tumor effect. This strategy will generate an outstanding accomplishment to optimizing anti-cancer performance by taking advantage of sonodynamic therapy together with anti-angiogenics in several different carcinomas.


Click reaction
DMF
TK-RB
TK-RB in DMSO
TK-RB in ACN
Absorbance
Wavelength (nm)
FL Intensity (a.u.)
Wavelength (nm)
Cell viability (% of control)
0.5 W/cm², 30 s
0.5 W/cm², 60 s
1 W/cm², 30 s
1 W/cm², 60 s
Control
US
0.5
1
2
4
8
TK-RB
VEGFR-1
ERK1/2 (44/42)
p-ERK1/2 (44/42)
β-actin
D
MCF-7
U87-MG
DCFH-DA (a.u.)
Control
US
TK-RB
SDT
1 μM
2 μM
4 μM
10 μM
U87-MG
MCF-7
Scale bar = 20 μM
U87MG
MCF-7
FL intensity (a.u.)
TK-RB (μM)
Control
US
TK-RB
SDT
U87MG
MCF-7
Scale bar = 100 μM

Poster Presentation : **ORGN.P-509**

Organic Chemistry

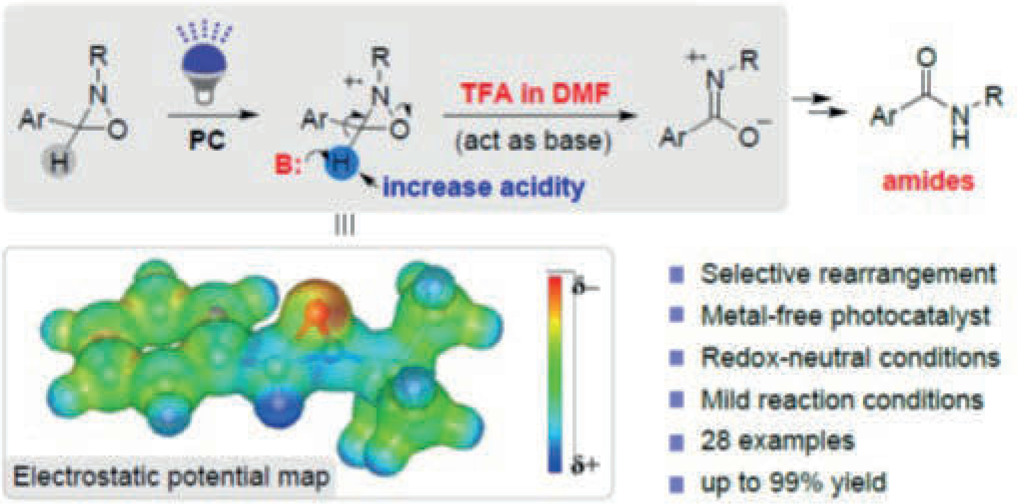
Exhibition Hall 1 FRI 11:00~12:30

Weak Base-Promoted Selective Rearrangement of Oxaziridines to Amides via Visible-Light Photoredox Catalysis

Sehoon Park, Ran Hui Kim, Jaehoon Jung*, Sang Kook Woo*

Department of Chemistry, University of Ulsan, Korea

Organic photocatalysts are recently receiving great attention in a variety of synthetic processes due to the advantages, such as energy saving, cost effectiveness, and environmentally friendliness. We present weak base-promoted selective rearrangement of oxaziridines to amides via visible-light photoredox catalysis, Acr^+-Mes which is a visible-light organic photocatalyst. The developed methods enable the preparation of various amides from oxaziridines with good functional group compatibility and good to excellent yields. The described approach has several advantages because it addresses the limitations of traditional methods by avoiding high-energy light sources and stoichiometric amounts of strong bases. Control experiments were performed to reveal the weak base-promoted (DMF or trifluoroacetate) selective rearrangement of oxaziridines to amides via single electron transfer (SET) mechanism. In addition, the density functional theory (DFT) calculations not only agree well with our experimental observations but also imply the importance of solvent components in controlling the reactivity of the photocatalytic SET process.



Poster Presentation : **ORGN.P-510**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Nanoliposome-encapsulated ratiometric fluorescent probe for detecting peroxynitrite flux

Minhyeok Choi, Youmi Choe, Ilwha Kim, Jungryun Kim, Yuvin Noh, Byungkook Kim, Saehee Rha, Zehra Zunbul, Jongseung Kim*

Department of Chemistry, Korea University, Korea

Peroxynitrite (ONOO−), a potent biological oxidant found in mitochondria, reacts with a variety of biomolecular targets in a variety of pathological environments, leading to a range of disease states. Herein, we designed a nanoliposome-encapsulated ratiometrically fluorescent probe (NRF) based on a hemicyanine structure Cy-O obtained through simple synthesis. As a result of the reaction with ONOO−, the oxidation and hydrolysis of a π-conjugation system within the nanoliposome causes a ratiometrically fluorescent response and a large-scale emission shift (238 nm), which provides a specific and sensitive method for the ONOO− detection. Furthermore, we used a suite of Gaussian 09 programs when DFT calculation has been performed at the 6-31+G(d,p) level to get insights into the chemical structure optical properties of Cy-O. Moreover, the practical applications of the nanoprobe to image exogenous and endogenous ONOO− were gloriously achieved further in live cells and animals.

Poster Presentation : **ORGN.P-511**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and stability of the luminescent europium chelates-based silica nanoparticles

Byeungjun Gong, Hoe In Kim, Chung-Min Park*

Chemistry, Gangneung-Wonju National University, Korea

In this work, we synthesized europium doped silica nanoshells particles with 160 nm diameters and tested their stability to develop the hybrid nanoplatforms for luminescent bio-labeling. Europium complexes with β-diketone-based ligands and modified 1,10-phenanthroline (phen)-based carboxylate ligands were synthesized. The europium doped SNPs exhibited a red emission at 615 nm on UV excitation. Time-dependent zeta potentials of the SNPs suspended in aqueous solution were characterized by dynamic light scattering. The surfaces and adhesion of the SNPs were observed by scanning electron microscopy measurements (SEM) and transmission electron microscopy (TEM), respectively. Results indicate that the SNP dopped with phen-based carboxylate ligand was the most stable SNP in aqueous media and the shape was not changed. A surface charge of -27 mV was achieved for the SNP, which assures a stable suspension in aqueous media.

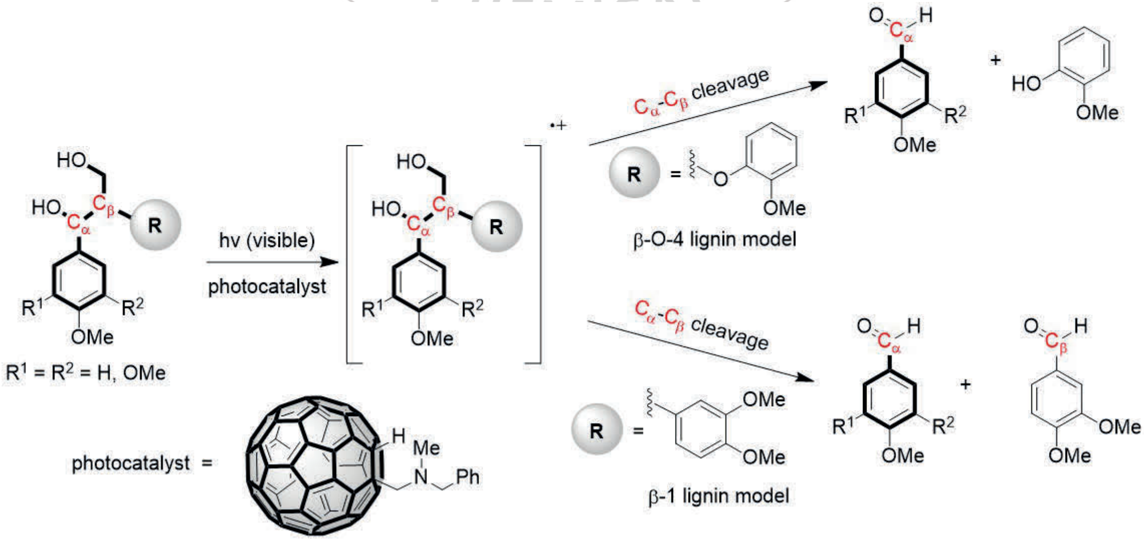
Poster Presentation : **ORGN.P-512**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Amine-Functionalized Fullerene-Sensitized Selective C-C Bond Cleavage Reactions of Lignin Model Substrates.

Suk Hyun Lim, Dae won Cho*

Department of Chemistry, Yeungnam University, Korea

Finding a selective and efficient fragmentation process under ambient condition is pivotal for the generation of fuels and chemical feedstocks from lignoceullosic biomass. In present study, visible-light and amine-functionalized fullerene based photocatalyst promoted photodegradation reactions of dimeric b-O-4 and b-1 lignin model compounds, containing varying number of methoxy substituent on the arene ring were explored to find and develop mild, eco-friendly photochemical techniques for efficient delignification. The results showed that, in contrast to well-known organic photoredox catalysts, amine-functionalized fullerene photocatalysts promoted photochemical reactions of lignin model compounds could lead to much efficient lignin fragmentation reactions through a pathway involving selective C_a-C_b bond cleavage process and, in addition, C_a- hydroxyl moiety within lignin model compounds played a significant role in the success of C_a-C_b bond cleavage reaction of lignin model substrates.



Poster Presentation : **ORGN.P-513**

Organic Chemistry

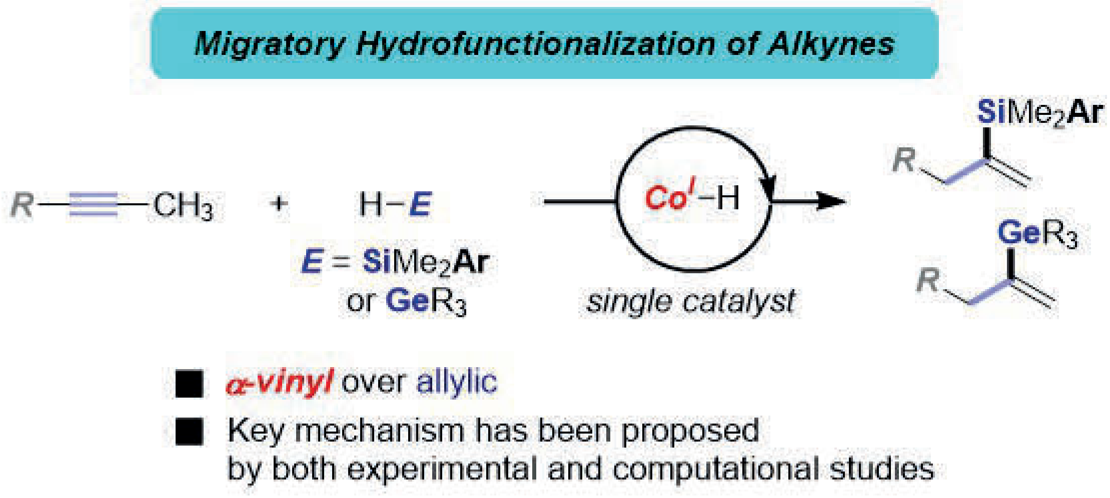
Exhibition Hall 1 FRI 11:00~12:30

Cobalt-catalyzed Regioselective Migratory Hydrofunctionalization of 2-Alkynes to Access α-Vinylsilanes and α-Vinylgermanes

Manoj Kumar Sahoo, Dongwook Kim[1], Sukbok Chang[2], Jung-Woo Park[*]

Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, Korea
[1]Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea
[2]Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Migratory hydrofunctionalization of alkynes are well studied using 2nd and 3rd-row transition metal catalysts which proceeds via a π-allyl metal intermediates however is unexplored under 1st-row transition metal catalysis. Herein we describe a cobalt-hydride catalytic system which can furnish α-vinylsilanes and α-vinylgermanes from 2-alkynes through alkyne π-bond migration. A cobalt-hydride species bearing a bulky ligand, bis(dicyclohexylphosphino)ethane enables the π-bond migration, and the key mechanism of the alkyne π-bond migration is strongly supported by both experimental and computational studies. In addition, the role of each reaction component for the unique α-vinyl selectivity is elucidated.



Poster Presentation : **ORGN.P-514**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A simple and efficient *in situ* generated copper nanocatalyst for stereoselective semihydrogenation of alkynes

ByoungYong Park, Min Su Han[1,*]

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

Development of a simple, effective, and practical method for (Z)-selective semihydrogenation of alkynes have been considered necessary for easy-to-access applications in organic laboratory scales. Herein, (Z)-selective semihydrogenation of alkynes was achieved using a copper nanocatalyst which was generated *in situ* simply by adding ammonia borane to an ethanol solution of copper sulfate. Different types of alkynes including aryl–aryl, aryl–alkyl, and aliphatic alkynes were selectively reduced to (Z)-alkenes affording up to 99% isolated yield. The semihydrogenation of terminal alkynes to alkenes and gram-scale applications were also reported. In addition to eliminating catalyst preparation, the proposed approach is simple and practical and serves as a suitable alternative method to the conventional Lindlar catalyst.

Poster Presentation : **ORGN.P-515**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Characterization of Indolizine Derivatives for Treatment of Cancer via synergistic STING activation

Eunsu Kim, Seulbi Lee, Sanghee Lee[1,*], Eunha Kim[*]

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

STING (Stimulator of interferon genes) has been emerged as a key mediator in the next generation of cancer immunotherapy to replace tumor immunophenotype from ‘cold’ to ‘hot’ via stimulation of innate immunity. Although the natural ligand or synthetic agonists for STING activate IFN-mediated immune response, promote anti-cancer immunity, and result promising pre-clinical outcome, however, intra tumoral administration and unfavorable pharmacokinetic properties have been issued for their clinical treatment. Therefore, there exists continuous effort to develop a combination therapy with synergistic effect for STING agonists. Here, we present synthesis and characterization of indolizine derivatives for immunotherapy of cancer via synergistic STING activation. To continue our endeavor for discovery of stimulator for STING activation, we conducted structure-activity relationship (SAR) study of indolizine scaffold to improve the immune modulation activity for STING-mediated innate immunity. Based on luciferase reporter gene assay, we confirmed a new indolizine compounds have the increased effect on activating STING pathway with the presence of cGAMP.

Poster Presentation : **ORGN.P-516**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

An analyte-triggered artificial peroxidase system based on dimanganese complex for a versatile enzyme assay

Suji Lee, Min Su Han*

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

This study described analyte-activatable artificial peroxidase system (caged Mn_2(bpmp)) by caging a dimanganese complex, exhibiting peroxidase-like activity, with analyte-reactive trigger. It allowed adjustments of the detection target to be applied depending on the trigger as well as the detection modes such as fluorescence and colorimetric as required. This system was successfully applied to a versatile enzyme assay for leucine aminopeptidase and γ-glutamyl transpeptidase based on spectrophotometric change induced from the oxidation of peroxidase substrate by analyte-triggered peroxidase-like activity.

Poster Presentation : **ORGN.P-517**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A β-Amyloid Selective Two-Photon Fluorescent Probe for Enhancing Signal-to-Noise Ratio via Twisted Intramolecular Charge Transfer

Byungkook Kim, Ilwha Kim, Yuvin Noh, Minhyeok Choi, Zehra Zunbul, Youmi Choe, Jungryun Kim, Saehee Rha, Jongseung Kim[*]

Department of Chemistry, Korea University, Korea

Alzheimer's disease(AD), which contains the most significant proportion of dementia, is a life-threatening neurodegenerative disease that eventually ends up with death. Several studies suggested that the aggregation of β-amyloid (Aβ) proteins is one of the major biomarkers for the development of Alzheimer's disease. Numerous diagnostic methods were invented to detect AD, and fluorescence imaging has been universally adopted to detect Aβ due to its advantages. As fluorescence technology advances, two-photon microscopy(TPM) has emerged as one of the most powerful instruments since its various benefits, for example, higher spatial resolution, three-dimensional imaging, lower tissue auto-fluorescence, etc. Despite the excellent sensing properties for Aβ, the latest two-photon fluorogenic probes, such as MeO-X04 and IBC2 could not be utilized in mouse study. MeO-X04 has poor blood-brain barrier (BBB) penetrability, and IBC2 has an off-target fluorescence issue which is usually observed in rigid "always-ON" type fluorescence. In this work, we designed a novel two-photon probe to redeem the previous probes. When the probe is excited, a twisted intramolecular charge transfer (TICT) state is populated and causes non-radiative relaxation. In contrast, when bounded to a protein target, the rotation is hindered, resulting in radiative relaxation. By the TICT process, the probe has an enhanced signal-to-noise (S/N) ratio. Besides, due to its lipophilicity and neutral properties, it maintains outstanding BBB penetrability and selectivity toward Aβ.

Poster Presentation : **ORGN.P-518**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Synthesis of 2-alkoxypyrimidines via Copper-mediated Oxidative Dehydrosulfurative Carbon-oxygen Cross-coupling of 3,4-Dihydropyrimidine-2-thiones with alcohols

Jihong Lee, Youjung Kwon[1,*], Jeong-Hun Sohn[*]

Department of Chemistry, Chungnam National University, Korea

[1]*chemistry department, Chungnam National University, Korea*

As well as being an integral part of DNA and RNA, the pyrimidine motif has been of interest to organic and medicinal chemists due to its diverse biological and pharmacological properties.[1] Comprehensive research on this privileged scaffold has generated dozens of commercial drugs. In particular, 2-aryloxypyrimidine compounds, such as bispyribac-sodium and pyriminobac-methyl as herbicides, and purmorphamine as an osteogenesis inducer have exhibited potent biological activity.[2] We present herein an aerobic Cu-promoted dehydrosulfurative carbon-oxygen cross-coupling with concomitant oxidative dehydrogenation of 3,4-dihydropyrimidin-1H-2-thiones (DHPMs) with alcohols. The reaction proceeded efficiently with diverse DHPMs and both aromatic- and aliphatic alcohols. Due to the ready availability of diverse DHPMs and alcohols,[3] the reaction method offers facile access to biologically and pharmacologically valuable 2-alkoxypyrimidine derivatives with rapid diversification.

References

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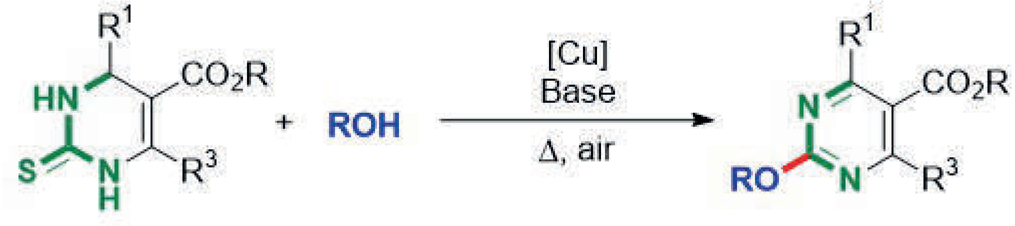
3.Singh, K.; Singh, K. Biginelli Condensation: Synthesis and Structure Diversification of 3,4-Dihydropyrimidin-2(1H)-one Derivatives. *Adv. Heterocycle.* Chem. **2012**, 105, 223-308.



R = aromatic, 1°,2° alkyl

Poster Presentation : **ORGN.P-519**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Formation of Metal-peptide frameworks through conformational adaptation of β-peptide foldamers

Seoneun Jeong, Jaewook Kim, Jintaek Gong[1], Yunho Lee[2], Kang Min Ok[3], Sunbum Kwon[4,*], Hee-Seung Lee[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Center for Multiscale Chiral Architectures, Korea Advanced Institute of Science and Technology, Korea*
[2]*Department of Chemistry, Seoul National University, Korea*
[3]*Department of Chemistry, Sogang University, Korea*
[4]*Department of Chemistry, Chung-Ang University, Korea*

Metal-coordinated frameworks fabricated from small peptidic ligands have recently received considerable attention owing to the vast structural and functional diversity of peptides. However, the rational design of metal-peptide frameworks remains elusive because of the intrinsic flexibility of peptides. β-Peptide foldamers with strong helical propensity can be the best alternative in this regard but have not been explored yet. In this presentation, we report the first metal-coordination-mediated assembly of β-peptide foldamers consisting of *trans*-2-aminocyclopentanecarboxylic acid (*trans*-ACPC) with 12-helical folding propensity. The coordination of Ag^+ to the terminal pyridyl moieties of short ACPC trimer and tetramer afforded a set of metal-peptide frameworks with unique topologies. Crystallographic analyses revealed that the formation of network structure was accompanied by notable conformational distortion from 12-helix to 8-helix. For the trimer, the formation of one-dimensional coordination polymers was observed when different solvents or counter anions were used.

Poster Presentation : **ORGN.P-520**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Maximizing the formation of strongly reducing radical anions for highly efficient purely organic photoredox catalysis and multiphoton excitation catalysis

Yonghwan Kwon, **Min Sang Kwon**[1,*]

Department of Materials Science and Engineering, Ulsan National Institute of Science and Technology, Korea

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

Efficient radical anion (PC•–) generation with strongly negative reduction potential of a organic photocatalyst (PC) is crucial for highly efficient photoredox catalysis and unconventional multiphoton excitation catalysis. However, conventionally, efficient formation of PC•– is only observed in PCs with less negative reduction potential and/or special conditions where back electron transfer to reducing agents can be avoided. Here, we report a novel strategy for highly efficient formation of PC•– with more negative reduction potential than conventional organic dyes. We observed that purely organic PCs with highly efficient generation of long-lived triplet excited states enable to efficiently produce PC•– even at very low catalyst loadings. With one of the PCs exhibiting a reduction potential of –1.66 V among the discovered PCs, successful reductive dehalogenations of activated aryl/alkyl halides were attained at extremely low PC loadings as low as 0.001 mol% with high oxygen tolerance, which is about two orders of magnitude lower than previously reported PCs. Notably, moderate to high yields were also achieved with higher PC loadings (0.5 – 5 mol%) for unactivated aryl/alkyl halides including unactivated aryl chlorides, which can be explained through unconventional consecutive photoinduced electron transfer process mediated by radical anions with highly negative excited state oxidation potential of –3.38 V.

Poster Presentation : **ORGN.P-521**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Helix Unwinding Property of β-Thiopeptide

Jungwoo Hong, Jintaek Gong[1], Jaewook Kim, Hee-Seung Lee[*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Center for Multiscale Chiral Architectures, Korea Advanced Institute of Science and Technology, Korea*

trans-ACPC(2-aminocyclopentanecarboxylic acid) is one of the most well-known β-amino acid, due to their helix inducing property. 12-membered intramolecular hydrogen bonding pattern of ACPC oligopeptide is almost absolute, no exceptions within our knowledge up to this day. These stable helical propensity makes ACPC oligopeptide as very useful building block of helical peptide, but on the other hand it also reduces structural and conformational diversity. Herein, we report a series of thioamide analogue of ACPC oligopeptide with designable and controllable conformation. Unlike ACPC oligopeptide with pentad repeat unit, triad repeat unit of cyclopentane side chains were observed on crystal structures when thioamide was introduced on N-terminus side. However, pentad repeat unit was maintained when C-terminus side was changed to thioamide. Since S atom is bigger than O, strain to helical winding makes tightly winded pentad repeat helix unwinding and become triad repeat helix.

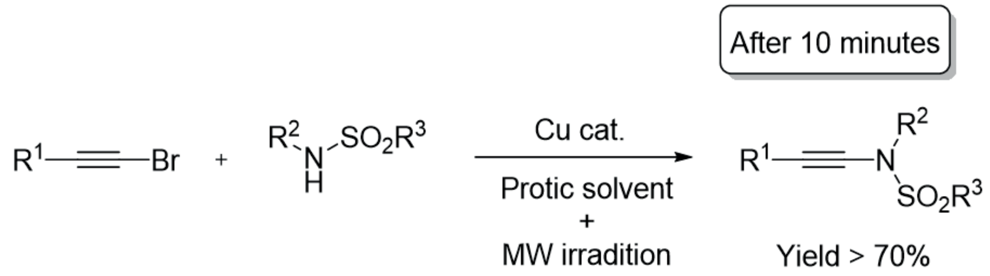
Poster Presentation : **ORGN.P-522**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Accelerated Cu-catalyzed Amidation of Alkynyl Bromide by Synergy of Solvent and Microwave : Rapid Synthesis of Sulfonamide substituted Ynamides

SuJeong Hong, Hyun-Suk Yeom[*]

Center for Eco-Friendly New Materials, Korea Research Institute of Chemical Technology, Korea

Ynamides are useful building blocks and have been widely used in synthetic chemistry. The strong polarization of the alkyne bond due to the presenced of *N*-atom allows ynamides to undergo highly efficient, regio- and stereoselective transformations. As a result of this increased interest for theses building blocks, there is a strong demand for the development of efficient, robust, and reliable methods for their synthesis. A general method for the preparation of ynamides is a transition metal such as Cu and Fe catalyzed C-N cross-coupling reaction between alkynes and amides. However, these methods require a long reaction time of 12 to 36 hours under heating conditions of more than 80 °C.Recently, our group discovered that using protic solvent under Cu-catalyzed condition dramatically reduced reaction time for the preparation of ynamide compared to the conventional methods. In addition, microwave irradiation more accelerates the reaction rate for amidation of alkynyl bromide to afford ynamides in 10 minutes. The details of the study are described in this presentation.



Poster Presentation : **ORGN.P-523**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of amphiphilic POSS (polyhedral oligomeric silsesquioxanes)-porphyrin nanomaterials for antimicrobial applications

Eunhee Jeoung*, Dongjin Kim[1], Minjae Seo[1], Hungyu Kang[1]

Department of Chemistry, Gangneung-Wonju National University, Korea
[1]*chemistry, Gangneung-Wonju National University, Korea*

Multidrug-resistant (MDR) biofilm formation of bacteria is challenging issue to the development of antimicrobial materials. Conventional antibiotics have some issue on penetration of those biofilms of bacteria for drug efficacy as well as fast emergence of new antibiotic-resistant bacteria. Overdose of antibiotics also cause the environmental water pollution problem in a long term. Light-based photodynamic antimicrobial approach has attracted by many researchers as alternatives to eradicating bacteria. Here we report the new type of antimicrobial nanomaterials based on porphyrin moiety which is compatible to the biological conditions and show low toxicity to mammalian cells. We have designed and synthesized the amphiphilic POSS (polyhedral oligomeric silsesquioxanes)-porphyrin materials for antibacterial applications. We also performed the studies of the efficient synthetic methodology of the targeted materials and their spectroscopic characteristics. Studies on their effective cellular uptake, toxicity evaluation and antibacterial therapeutic potential will be examined in near future.

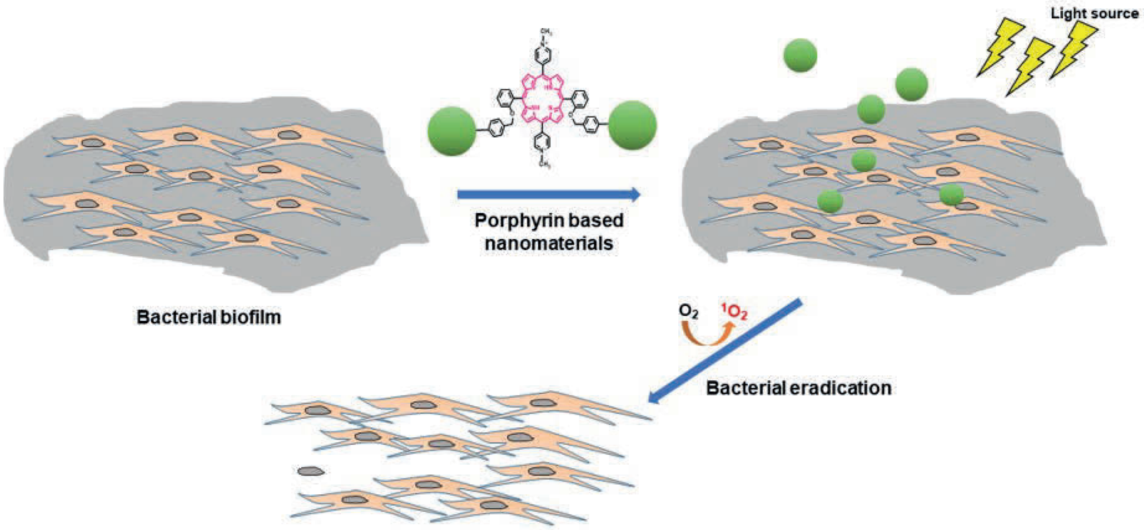


Figure 1. Antimicrobial photodynamic therapy

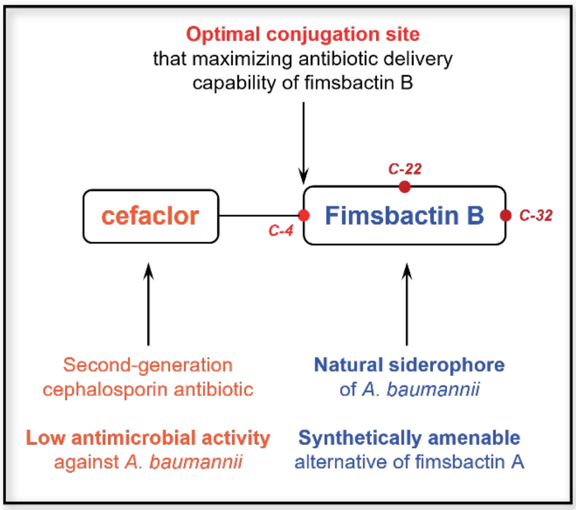
Poster Presentation : **ORGN.P-524**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Total Syntheses of Fimsbactin B-Cefaclor Conjugates and Evaluation of Antimicrobial Activity

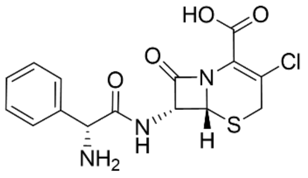
Do Young Kim, Hak Joong Kim*

Department of Chemistry, Korea University, Korea

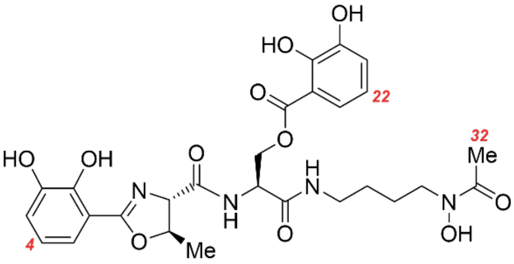
Acinetobacter baumanii is a gram-negative bacterium belonging to ESKAPE pathogens, whose extensive antibiotic resistance is posing serious threats to the human welfare. As the antibiotic resistance of *A. baumannii* is often associated with the reduction in the outer membrane permeability, a strategy based on intracellular delivery of an antibiotic molecule via siderophore uptake machineries that are responsible for active iron uptake has been attracting great interests. Fimsbactin is one class of the natural siderophores of *A. baumannii*, among which fimsbactin A is the predominant factor in the *A. baumannii* culture isolates. Total synthesis of fimsbactin A was found to be demanding due to facile epimerization of a stereogenic center, and therefore it was not suitable to utilize as an antibiotic delivery vehicle. To find a synthetically amenable alternative, we synthesized other fimsbactin variants and tested their siderophore activities to reveal that fimsbactin B can be a faithful alternative of fimsbactin A.To test whether fimsbactin B can function as a drug delivery vehicle targeting *A. baumannii*, several conjugates linked with cefaclor, a second-generation cephalosporin, were prepared. Since the identification of an appropriate conjugation site not interfering with the interaction between a siderophore-antibiotic conjugate and the cognate uptake machinery was critical for the optimal cellular delivery, three different sites, C-4, C-22, and C-23, were modified. The activity assay revealed that all conjugates are dramatically more potent than cefaclor alone, among which the C-4 conjugate variant exhibits the highest activity. This result clearly demonstrates that the fimsbactin-based antibiotic delivery can be an effective approach for overcoming the antibiotic-resistance of *A. baumannii*.



Synthetic design of fimsbactin B-cefaclor conjugates



Cefaclor



Fimsbactin B

Poster Presentation : **ORGN.P-525**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Antiviral effects of phenolic amides derivatives from tobacco leaves

Seokyun Sa, Jeong Tae Lee*

Chemistry, Hallym University, Korea

Phenolic compounds, which are one of the secondary metabolites of plants, have significant physiological and morphological values. Phenolic compounds are involved in plant development and reproduction processes and have anti-inflammatory, antioxidant and anti-allergic effects in humans. Among the phenolic amides extracted from tobacco leaves, tabamides A-C have been reported to have antiviral effects against the tobacco mosaic virus. In this study, the design and synthesis of derivatives of tabamide A were carried out, and the antiviral effect against influenza virus A was evaluated. Most of the derivatives showed a better response in antiviral effects, suggesting new leads for antiviral agents.

Poster Presentation : **ORGN.P-526**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis of Novel Tetracyclic Pyrazolidinones from [3 + 2] Cycloaddition of N-Silyl Enamines and Azomethine Imines.

Vinh Do cao, Seewon Joung[1,*]

Department of Chemistry, Mokpo National University, Vietnam
[1]*Department of Chemistry, Mokpo National University, Korea*

Enamines are well-known as versatile structural motifs in organic synthesis which can be converted to various natural and pharmaceutical structures like amines, amidines and N-heterocycles. The recent research about hydrosilylation showed quinolines and isoquinolines were mildly reduced under borane-catalyzed hydrosilylation condition to accumulate endo N-silyl enamines as intermediates. In our previous research, we also utilized this intermediate to produce the corresponding cyclic amidines via a cycloaddition pathway. Herein, we continued this idea using N-silyl enamines from borane-catalyzed hydrosilylation as a precursor to develop the new synthetic strategies furnishing tetracyclic pyrazolidinones based on [3 + 2] cycloaddition with azomethine imines.

Poster Presentation : **ORGN.P-527**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Ligand Modifications Enable Catalytic Diastereo- and Enantioselective Olefin Difunctionalizations

Suhyeon Kim, Dongwook Kim[1], Seung Youn Hong[2,*], Sukbok Chang[1,*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*
[2]*Department of Chemistry, Massachusetts Institute of Technology, United States*

Among the central themes in synthetic chemistry is the development of a novel strategy to attain more efficient and mild reactions and to expand the chemical space for asymmetric catalysis. Herein, we describe how catalytic alkene difunctionalizations can be achieved through acylnitrenoid transfer by harnessing the system of Cp*Ir(κH^2-LX), which cannot previously yield the catalytic process. A key strategy is tuning the orbital symmetry of Ir-nitrenoid intermediates upon ligand design for achieving two special goals: (i) bypassing the catalyst degradation via the concerted ligand-participation and (ii) delivering fundamentally new reactivity by altering the mechanistic pathway to involve stepwise nitreneoid transfer and nucleophile insertion. Based on the inspiration from FMO analysis, we systemically tailored an effective catalyst that can produce a range of difunctionalized lactams with a broader generality in terms of nucleophiles. The reaction is highly stereoselective, which is proposed to originate from a ligand nucleophile interaction as supported by our computation. The current mechanistic platform also enabled the invention of asymmetric methods for introducing two-point chirality in (oxy-alkyl) lactams for the first time with excellent enantioselectivity of up to >99:1 e.r.

Poster Presentation : **ORGN.P-528**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Disengaging Aromatics with Triazole-Fused Iptycenes.

Hongsik Kim, Dongwhan Lee[1,*]

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

In the condensed phase, molecules tend to aggregate to avoid unfilled space. For aromatic molecules, π–π stacking is one of the main intermolecular interactions. In the field of porous materials and solid-state fluorophores, it is necessary to prevent such π-stacking. Iptycenes with rigid propeller-shaped structures have been ingeniously used for such purpose. However, existing methods to introduce iptycene moieties are limited to condensation reactions or Diels-Alder reactions, which lack general applicability. We suggest a rational approach to destack aromatic molecules by installing 1,2,3-triazole fused iptycene, triazoliptycene (TI). Our general method exploits the following two facts. First, unlike other heteroaromatic-fused iptycenes, TI have a nitrogen atom that can engage in C–N cross-coupling reactions. Second, tight intramolecular C–H···N hydrogen bonds between triazole nitrogen and aromatic hydrogen atoms enforce the coplanarity of the triazole–aryl unit despite that the C–N single-bond junction is free to rotate. This planar geometry is critical for suppressing extensive intermolecular contacts. As a proof-of-concept, we have introduced multiple TI units to various aryl halides. In the condensed phase, π-π interactions are effectively suppressed as confirmed by single-crystal X-ray crystallography. Especially, tetra(triazoliptycylphenyl)ethane (TTPE) features large void volume (27.2% per unit cell) and highly bright solid-state florescence, which can be modulated by mechanical stress and vapor uptake. In this presentation will be discussed key design principles and synthetic strategies to disengage rigid 3D aromatics in the condensed phase to program stimuli-responsive light-emitting properties.

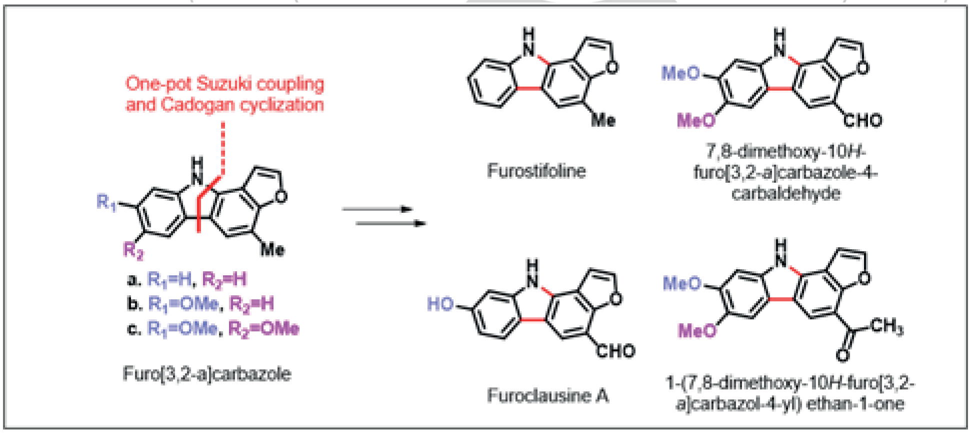
Poster Presentation : **ORGN.P-529**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Total Synthesis of Furo[3,2-a]carbazole Alkaloids

Shafrizal Rasyid Atriardi, Sang Kook Woo*

Department of Chemistry, University of Ulsan, Korea

Furo[3,2-a]carbazole is a hetero-annulated carbazole with furan ring attached on carbazole core ring and remarkably diverse family of natural products. Furo[3,2-a]carbazole mostly isolated from plants of the genus Murraya, Glycosmis, and Clausena from the family Rutaceae. Herein, an early stages synthesis of 7-methylbenzofuran moiety from commercially available o-cresol following by a short, efficient, and divergent synthetic approach to four furo[3,2-a]carbazole alkaloids, namely furostifoline, furoclausine A, and two un-named furo[3,2-a]carbazole alkaloids has been developed with the integration of one-pot Suzuki coupling and Cadogan cyclization as a key step.



Poster Presentation : **ORGN.P-530**

Organic Chemistry

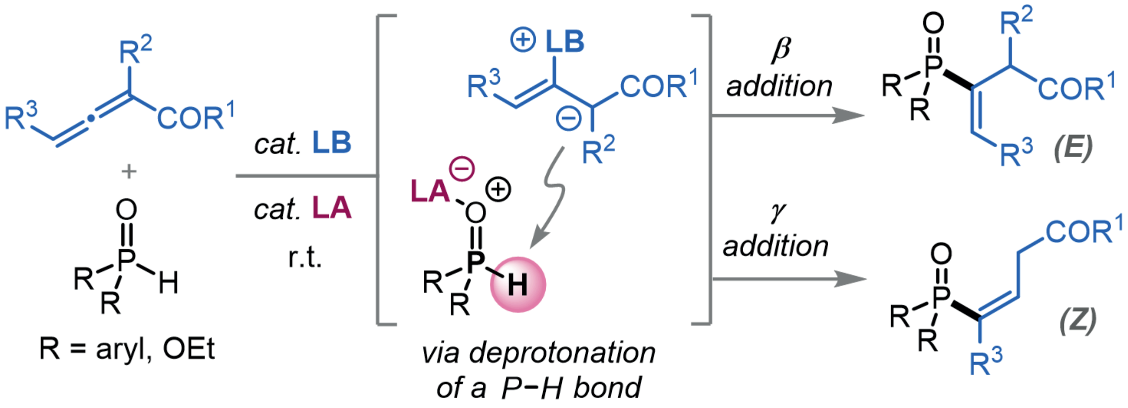
Exhibition Hall 1 FRI 11:00~12:30

Regio- and Stereoselective Addition of Secondary Phosphine Oxides to Allenoates Catalyzed by Main Group Lewis Pairs

Soojin Kwak, Sarah Yunmi Lee*

Department of Chemistry, Yonsei University, Korea

Alkenylphosphorus compounds are versatile building blocks for the preparation of a variety of organophosphorus structures that are widely applied in the fields of synthetic, agrochemical, and medicinal chemistry. Although addition of phosphorus nucleophiles to electron-deficient allenes could potentially provide an efficient route to such compounds, the development of atom-economical, regio- and stereoselective processes of this type has remained a significant challenge. In this presentation, we establish the synergistic, boron-Lewis acid/phosphine-Lewis base catalyzed method for the hydrophosphinylations of multisubstituted allenoates with secondary phosphine oxides (SPOs) that occurs with high regio- and stereoselectivity. This process proceeds under mild conditions and allows the atom-economical generation of alkenylphosphorus products. Mechanistic investigations including kinetic and spectroscopic studies revealed that the P–H bond of SPOs was cleaved by the cooperative action between $B(C_6F_5)_3$ and a phosphonium zwitterion as a Brønsted base generated by the addition of $P(4\text{-}OMeC_6H_4)_3$ to allenoates in the rate-determining step. We also show that this process could proceed efficiently on a gram-scale and that the products could be derivatized into other useful organophosphorus compounds.



Main group catalysis • Regioselective • Stereoselective • 100% Atom economy

Poster Presentation : **ORGN.P-531**

Organic Chemistry

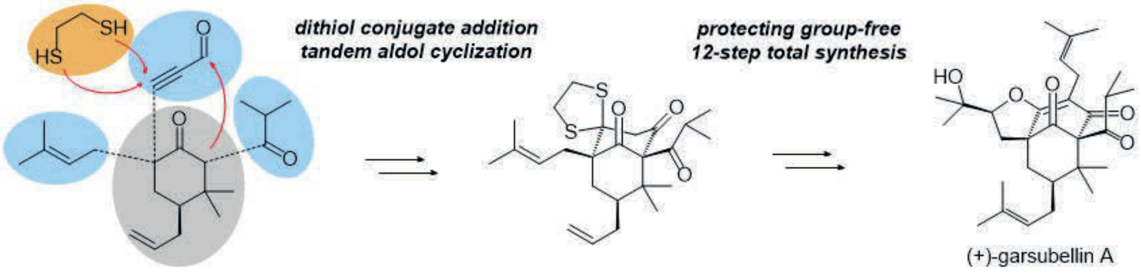
Exhibition Hall 1 FRI 11:00~12:30

Enantioselective Total Synthesis of (+)-Garsubellin A

Minchul Choi, Chulbom Lee*

Division of Chemistry, Seoul National University, Korea

Garsubellin A is a meroterpene capable of enhancing the enzyme choline acetyltransferase whose decreased level is believed to play a central role in the symptoms of Alzheimer's disease. Due to the potentially useful biological activity together with the novel bridgedand fused cyclic molecular architecture, garsubellin A has garnered substantial synthetic interest, but its absolute stereostructure has been undetermined. In this poster, the first enantioselective total synthesis of (+)-garsubellin A. Our synthesis relies on stereoselective fashioning of a cyclohexanone framework and double conjugate addition of 1,2-ethanedithiol that promotes aldol cyclization to build the bicyclic [3.3.1] skeleton. The twelve-step, protecting group-free synthetic route has enabled the syntheses of both the natural (–)-garsubellin A and its unnatural (+)-antipode for biological evaluations.



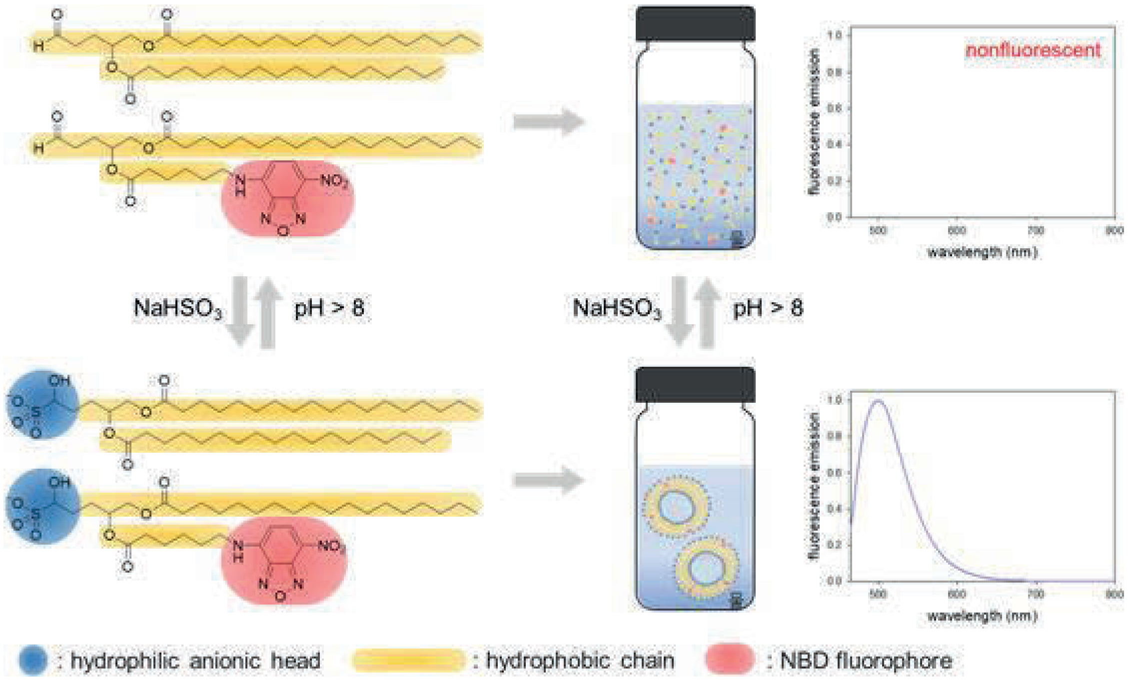
Poster Presentation : **ORGN.P-532**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Design, synthesis, and analysis of pH-responsive surfactant: α-hydroxy sulfonate-based non-phospholipid

Minseo Kang, Bongjin Moon*

Department of Chemistry, Sogang University, Korea

Surfactants, also called surface-active agents, have a hydrophilic head group soluble in water and a hydrophobic tail soluble in oil. A “smart surfactant” is a nonpolar molecule that becomes an amphiphilic surfactant by an external stimulus. The stimuli can be pH, CO2, redox, temperature, light, magnetic fields, or complex formation. We designed a pH-responsive surfactant based on the well-known aldehyde/bisulfite to α-hydroxysulfonate equilibrium. The surfactant is a non-phospholipid composed of a hydroxy sulfonate head group and two long hydrocarbon tails. Under neutral conditions, it acts as an anionic surfactant, forming bilayer vesicles. Under basic conditions, however, it destabilizes the vesicles by returning to aldehyde form.In addition, we synthesized a fluorescent lipid probe containing a nitrobenzoxadiazole (NBD) group. Because NBD has different fluorescence depending on the polarity of the environment, the formation of bilayer vesicles can be easily observed through monitoring the fluorescence emission.


nonfluorescent
fluorescence emission
wavelength (nm)
NaHSO$_3$
pH > 8
NaHSO$_3$
pH > 8
fluorescence emission
wavelength (nm)
NO$_2$
NH
OH
: hydrophilic anionic head
: hydrophobic chain
: NBD fluorophore

Poster Presentation : **ORGN.P-533**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Allosterically Gated Molecular Actuator Built on Canopied Calix[4]arene

Taewon Kang, Dongwhan Lee*

Division of Chemistry, Seoul National University, Korea

Machines operate by interdependent moving parts that transmit or amplify directional motions. Nature utilizes similar strategies to relay signaling events over a long distance in a cascade fashion. As a functional mimic of allosterically gated biological machinery, we have built a canopied calix[4]arene system that relays binding events at one side of the molecule to the gate opening and closing motions at the other side of the molecule. As mechanically coupled canopy units, propeller-shaped triazolitpycene fragments were installed through C–N single bonds, the rotational freedom of which was effectively regulated by tight intramolecular C–H···N hydrogen bonds to produce the desired capped structure. A combination of 1H NMR spectroscopic titration and single-crystal X-ray diffraction (SC-XRD) studies with small amines and related Brønsted bases revealed that host-guest interactions at the lower rim of the molecular basket could propagate mechanically to the upper rim to drive gate opening and closing motions. This presentation will discuss key design principles, synthetic implementations, and experimental/computational studies on the molecular mechanisms of allosterically controlled molecular actuation.

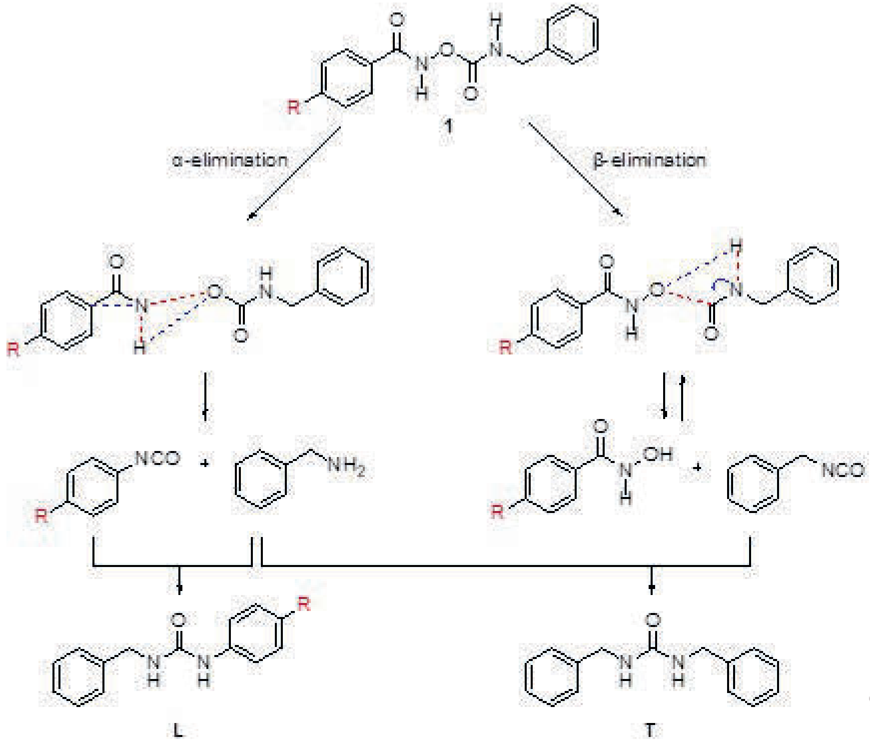
Poster Presentation : **ORGN.P-534**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Substituent effect of O-(benzylcarbamoyl)benzohydroxamtes on their fragmentation-recombination pathways

Youngchan Bang, Bongjin Moon[1,*]

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

O-carbamoylhydroxamates are generally known to give the corresponding isocyanates via Lossen rearrangements. However, chemists have paid little attention to the detailed reaction pathways of O-carbamoylhydroxamate depending on its structural variations. Moreover, only a few articles have been reported for non-Lossen type rearrangement of O-carbamoyl hydroxamates. In this perspective, we have synthesized several O-carbamoyl hydroxamates and systematically investigated the substituent effect on the possible reaction pathways.O-(benzylcarbamoyl)benzohydroxamtes with p-substituted benzoyl group (1) were prepared from the corresponding dioxazolones. The dioxazolone precursors were synthesized with hydroxamic acid and phosgene derivatives. To investigate the p-substituent effect on the fragmentation-recombination reaction, we have heated 1 and analyzed the resulting products by NMR spectroscopy. In most cases, two ureas, L and T, were observed in different ratios depending on the p-substituent. The proposed mechanism starts with α- and β- elimination of 1. As increasing the electron-donating ability of the substituent, Lossen rearrangement would be dominated, providing urea L as the primary product. If not, thermal decomposition would give urea T. Interestingly, despite the unignorable amount of H2O in DMSO-d6, only two types of urea were observed, not four types. The Hammett plot showed a linear relationship between product ratio (L/T) and the substituent constants (σp). This linearity means the ratio of L/T is mainly affected by the p-substituent. The kinetic data of the experiments showed that the reaction follows the first-order at 0.1 mM concentration.


1
α-elimination
β-elimination
R
NCO
NH2
OH
L
T

Poster Presentation : **ORGN.P-535**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Enhancing the Cytotoxicity of Reactive Oxygen Species in Hypoxic Tumor by conjugating An Ethacrynic Acid with BODIPY-Based Photosensitizer

Jieun Lee, Jungryun Kim, Ilwha Kim, Yuvin Noh, Saehee Rha, Zehra Zunbul, Minhyeok Choi, Byungkook Kim, Youmi Choe, Jongseung Kim[*]

Department of Chemistry, Korea University, Korea

Despite being clinically approved for cancer treatment, photodynamic therapy (PDT) still suffers from limitations. One of the major limitations is mostly oxygen dependent. This reduces the efficacy of PDT in hypoxic tumors, as cytotoxic reactive oxygen species (ROS) are less generated in regions of low oxygen tension. Glutathione-pi (GST-pi) is a crucial enzyme that protects cells from apoptosis caused by ROS. We develop a newly designed photosensitizer which contains both a brominated BODIPY and an ethacrynic acid as GST-pi inhibitor. The combination of ROS generation and GST-pi inhibition leads to a synergistic anticancer effect when this photosensitizer is photoirradiated. Compared to BODIPY-based photosensitizer alone, cell-killing effect is improved under hypoxic conditions both in vitro and in vivo. We conclude that enhanced therapeutic PDT outcomes can be achieved even under hypoxia by better use of available oxygen in the tumor environment.

Poster Presentation : **ORGN.P-536**

Organic Chemistry

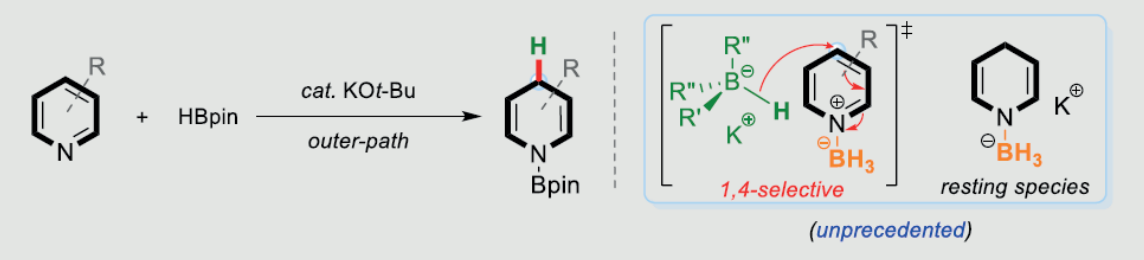
Exhibition Hall 1 FRI 11:00~12:30

Alkoxide-Promoted Selective Hydroboration of *N*-Heteroarenes: Pivotal Roles of *in situ* Generated BH_3 in the Dearomatization Process

Eunchan Jeong, Joon Heo, Sukbok Chang*

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

While numerous organo(metallic)catalyst systems were documented for dearomative hydroboration of *N*-aromatics, alkoxide base catalysts have not been disclosed thus far. Described herein is the first example of alkoxide-catalyzed hydroboration of *N*-heteroaromatics including pyridines, providing a broad range of reduced *N*-heterocycles with high efficiency and selectivity. Mechanistic studies revealed an unprecedented counterintuitive dearomatization pathway, in which (i) pyridine-BH_3 adducts undergo a hydride attack by alkoxyborohydrides, (ii) *in situ* generated BH_3 serves as a catalytic promoter, and (iii) 1,4-dihydropyridyl borohydride is in a predominant resting state.



Poster Presentation : **ORGN.P-537**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

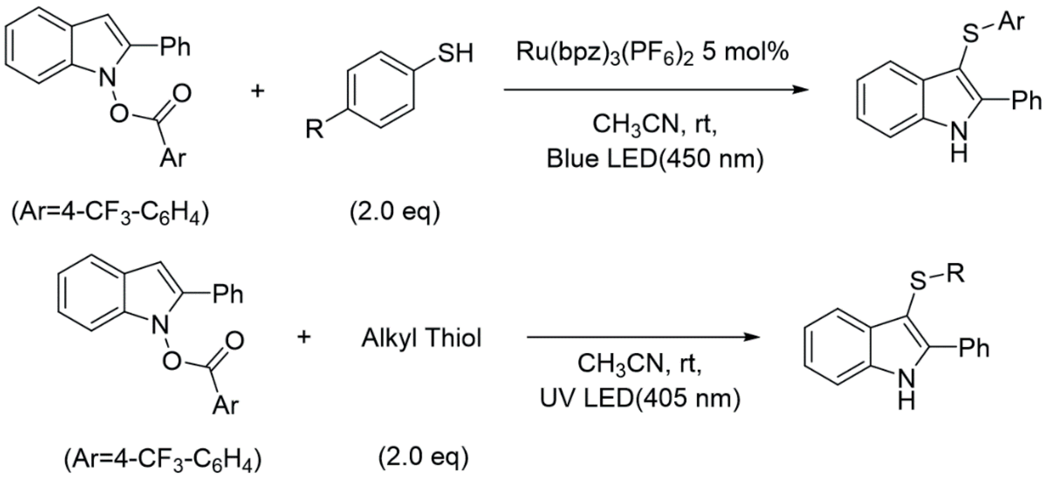
C-H Sulfenylation of Umpoled Indoles under Photocatalytic condition.

Chul yong Lee, Seunghoon Shin[1,*]

Department of Chemistry, Hanyang university, Korea
[1]*Department of Chemistry, Hanyang University, Korea*

Drugs containing 3-sulfenylindoles have diverse pharmaceutical profile, and diverse synthetic routes have been developed, frequently involving RSX agents (X = SR or NR$_2$).[1] Thiols (ArSH or AlkSH)2 has also been utilized as C-H coupling partners using external oxidants.[2] Recently, we developed N-hydroxyindole derivatives for C-H arylation,[3] and we wondered whether this umpoled indoles could be used in the C-H sulfenylation. Under the irradiation of blue LEDs employing Ru(bpz)$_3$ as the photocatalyst, N-acyloxyindole derivatives underwent efficient sulfenylation with aromatic thiols at C3. This photocatalytic conditions gave superior yield than either Brønsted acid or Cu-catalysis.[3b] The working hypothesis involves energy transfer (EnT) to form a carboxy radical, formation of a thiyl radical, and its addition into a N-acyloxyindole. For aliphatic thiols having higher S-H bond strength, an alternative condition was developed involving UV photolysis in the absence of catalyst.

References
1. (a) Liu, C. -R.; Ding, L. -H. *Org. Biomol. Chem.* 2015, 13, 2251; (b) Tudge, M.; Tamiya, M.; Savarin, C.; Humphrey, G. R. *Org. Lett.* 2006, 8, 4, 565–568; (c) Yang, F.-L.; Tian, S.-K.; *Angew. Chem. Int. Ed.* 2013, 52, 4929 –4932.2. (a) Maeda, Y.; Koyabu, M.; Nishimura, T.; Uemura, S.; *J. Org. Chem.* 2004, 69, 7688-7693; (b) Yadav, J. S.; Reddy, B. V. S.; Reddy, Y. J.; *Tetrahedron Letters* 2007, 48, 7034–7037. (c) Guo, W.; Tan, W.; Zhao, M.; Tao, K.; Zheng, L.-Y.; Wu, Y.; Chen, D.; Fan, X.-L.; *RSC Adv.*, 2017, 7, 377393. (a) Oh, S. M. ; Shin, S. *Bull. Korean Chem. Soc.* 2021, 42, 925; (b) Oh, S. M.; N. H. Nguyen; Shin, S. *manuscript in preparation.*


Ph
N
O
O
Ar
(Ar=4-CF$_3$-C$_6$H$_4$)
+
SH
R
(2.0 eq)
Ru(bpz)$_3$(PF$_6$)$_2$ 5 mol%
CH$_3$CN, rt,
Blue LED(450 nm)
S
Ar
Ph
N
H
Ph
N
O
O
Ar
(Ar=4-CF$_3$-C$_6$H$_4$)
+
Alkyl Thiol
(2.0 eq)
CH$_3$CN, rt,
UV LED(405 nm)
S
R
Ph
N
H

Poster Presentation : **ORGN.P-538**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Enantioselective Access to Spirolactams via Nitrenoid Transfer Enabled by Enhanced Noncovalent Interactions

Euijae Lee, Yeongyu Hwang[1], Yeong Bum Kim, Dongwook Kim[1], Sukbok Chang[1,*]

Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea
[1]*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

Described herein is the Ir-catalyzed enantioselective access to chiral spirolactam products via the nitrenoid transfer to aromatic ipso-carbons. The key strategy for precise stereocontrol is to enhance the secondary attractive and repulsive interactions between the chiral catalyst and substrates by the introduction of a traceless O-silyl achiral auxiliary, thus effectively differentiating two prochiral faces of arenol-derived 1,4,2-dioxazol-5-one substrates.

Enantioselective Access to Spirolactams via Nitrenoid Transfer Enabled by Enhanced Noncovalent Interactions

Euijae Lee†, Yeongyu Hwang†, Yeong Bum Kim, Dongwook Kim, and Sukbok Chang*

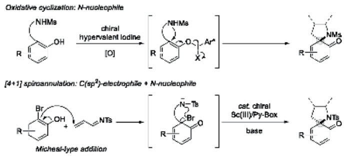
Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, KOREA
Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science (IBS), Daejeon 34141, KOREA

E-mail : ejlk12@kaist.ac.kr

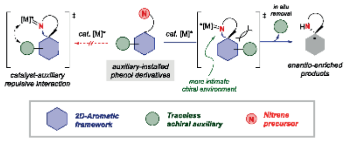
[†] These authors contributed equally to this work

Introduction

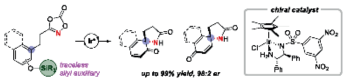
Previous Works
C-N Bond-Forming Asymmetric Spirocyclization



Our Strategy
Harnessing Ir-Nitrenoid & Traceless Achiral Auxiliary

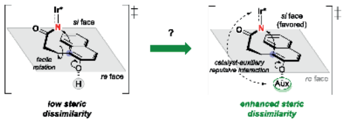


Asymmetric Synthesis of Spirolactams Achieved by Enhanced Noncovalent Interactions

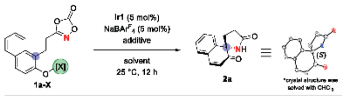


- First example of enantioselective spirolactam synthesis via Ir-nitrenoid transfer
- Bulky O-silyl auxiliary enhances the substrate/catalyst secondary interactions
- Operates in both *ortho-* and *para-*dearomatizations

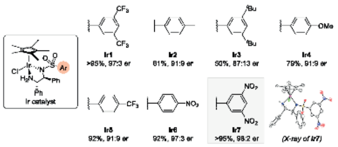
Working Hypothesis



Reaction Optimization

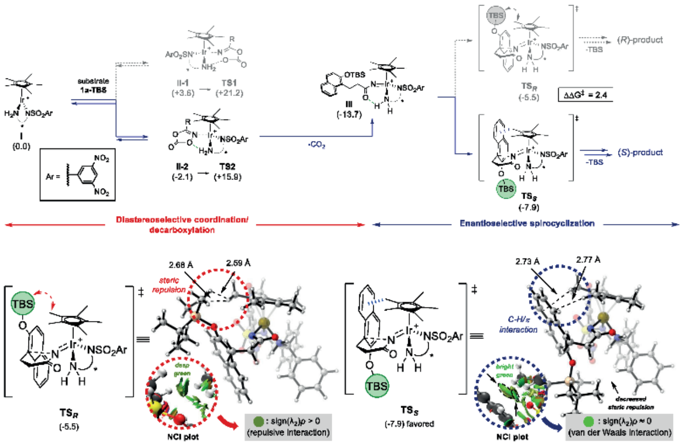


entry	[X]	solvent (M)	additive (equiv)	yield (%)	er
1	H	HFIP (0.1)	-	30	47:53
2	TIPS	HFIP (0.1)	-	79	92:8
3	TBS	HFIP (0.1)	-	82	93:7
4	TBDPS	HFIP (0.1)	-	79	53:47
5	TBS	NFTB (0.1)	-	89	95:5
6	TBS	NFTB (0.1)	H_2O (5)	>95	95:5
7	TBS	NFTB (0.1)	H_2O (1)	>95	95:5
8	TBS	NFTB (0.5)	H_2O (1)	>95	97:3

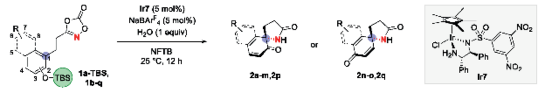


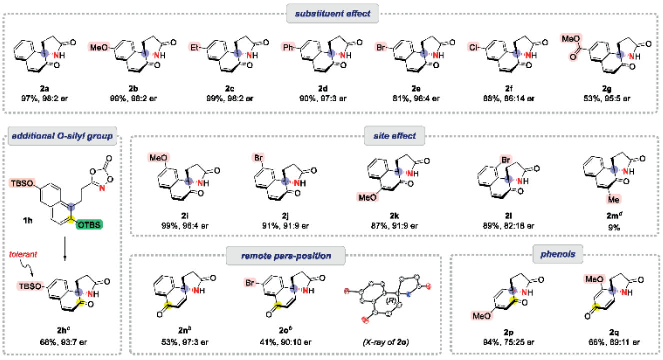
Ir1 >95%, 97:3 er
Ir2 81%, 91:9 er
Ir3 50%, 87:13 er
Ir4 79%, 91:9 er
Ir5 92%, 91:9 er
Ir6 92%, 97:3 er
Ir7 >95%, 98:2 er

Computational Analysis



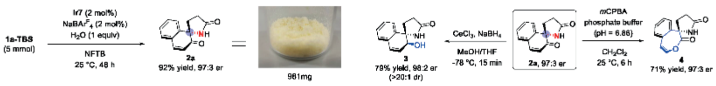
Reaction Scope





2a 97%, 98:2 er
2b 99%, 98:2 er
2c 99%, 98:2 er
2d 90%, 97:3 er
2e 81%, 96:4 er
2f 88%, 86:14 er
2g 53%, 95:5 er
2h^c 68%, 93:7 er
2i 99%, 96:4 er
2j 91%, 91:9 er
2k 87%, 91:9 er
2l 89%, 82:18 er
2m^d 9%
2n^b 53%, 97:3 er
2o^b 41%, 90:10 er
2p 94%, 75:25 er
2q 66%, 89:11 er

Synthetic Applications



Conclusion

- ❖ ***Construction of chiral tetrasubstituted stereocenter bearing amide functionality***
- ❖ ***Enhanced substrate/catalyst interactions enabled by traceless achiral auxiliary***
- ❖ ***Operation in both ortho- and para-dearomatization***

Lee, E.†, Hwang, Y.†, Kim, Y. B., Kim, D., Chang, S.* *J. Am. Chem. Soc.*, **2021**, *in revision*

Poster Presentation : **ORGN.P-539**
Organic Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Studies for sulfur containing detergents

Hyun Sung Lee, Pil Seok Chae[1,*]

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

Sulfur-containing compounds have received considerable interests in their synthesis and utilities. Sulfoxide group-bearing amphiphilic compound are especially notable due to their ability to form self-assemblies in aqueous solution. The dipole moment and dielectric constant of sulfoxide group are much larger than those of related functional groups such as sulfide or carbonyl groups. In addition, sulfoxide group can be reduced into sulfide group and the opposite conversion is also readily attained by oxidation. Thus, we introduced a sulfoxide group into the alkyl chain of dodecyl maltoside (DDM), a widely used detergent for membrane protein study. We prepared several DDM analogues with different locations of the sulfoxide group within the detergent alkyl chain. When self-assemblies formed by these DDM analogues were investigated in terms of CMC and micelle size, a couple of detergents with the sulfoxide group at the specific location of the alkyl chain gave relative low CMCs compared to the other analogues. This result indicates that these low CMC detergents form the dipole-dipole interactions between detergent molecules under micellar environments. The resulting micelles with enhanced stability could be favorable for membrane protein stabilization.

Poster Presentation : **ORGN.P-540**

Organic Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Hydrophosphorylation of *N*-Heteroaryl-Substituted Alkenes by Boron-Lewis Acid Catalysis

Choi JeongIn, Sarah Yunmi Lee*

Department of Chemistry, Yonsei University, Korea

In this poster, we describe the boron Lewis acid-catalyzed hydrophosphorylations of *N*-heteroaryl-substituted alkenes with dialkylphosphonates. This atom-economical process proceeds under mild conditions and occurs with various alkenes, thereby generating an array of phosphorus-containing *N*-heterocycles in good to excellent yields. The available mechanistic data can be explained by the pathway wherein the P-H bond of dialkylphosphonates is cleaved by the synergistic action of a boron catalyst and a basic *N*-heterocyclic moiety of the alkene substrate. The resulting phosphinite anion serves as a phosphorus nucleophile for the conjugate addition to the alkenes.

Poster Presentation : **MEDI.P-541**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Cholinesterase inhibitory activity of alpha-lipoic acid-piperidine thioacetal compounds

Ji hyun Hwang*, **Jiyeon Lee, GaHyun Park, Eunseo Jeon, Yeonsoo Kim, Jeong Ho Park***, **Byong Wook Choi**[1], **Bong Ho Lee**[2]

Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea
[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*
[2]*Department of Chemical and Biological Engineering, Hanbat National University, Korea*

Based on the cholinergic theory for the treatment of Alzheimer's disease (AD), we reported the amide derivatives of lipoic acid and piperidine had an inhibitory effect on acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE). alpha -Lipoic acid (ALA) is a fatty acid produced in small amounts in the human body. It is an essential reporting factor for mitochondrial respiratory enzymes and improves mitochondrial function. ALA is well known as an antioxidant and has further beneficial effects on neurodegenerative diseases such as AD, Parkinson's disease, and Huntington's disease. ALA has disulfide bonds and can be reduced to dithiol. In this study, the disulfide bond of the ALA-piperidine amide derivative was converted into thioacetal compounds. Various benzaldehyde compounds were used to synthesize thioacetal compounds. The relationship between the structure and the inhibitory activity on cholinesterase was investigated using the synthesized lipoic acid-piperidine thioacetal compounds. Compounds 32 ($IC_{50} = 0.49 \pm 0.05 \mu M$ for AChE, $IC_{50} = 0.15 \pm 0.008 \mu M$ for BuChE) showed better inhibitory activity than the positive control, galantamine ($IC_{50} = 1.70 \pm 0.9 \mu M$ for AChE, $IC_{50} = 9.4 \pm 2.5\ \mu M$ for BuChE).

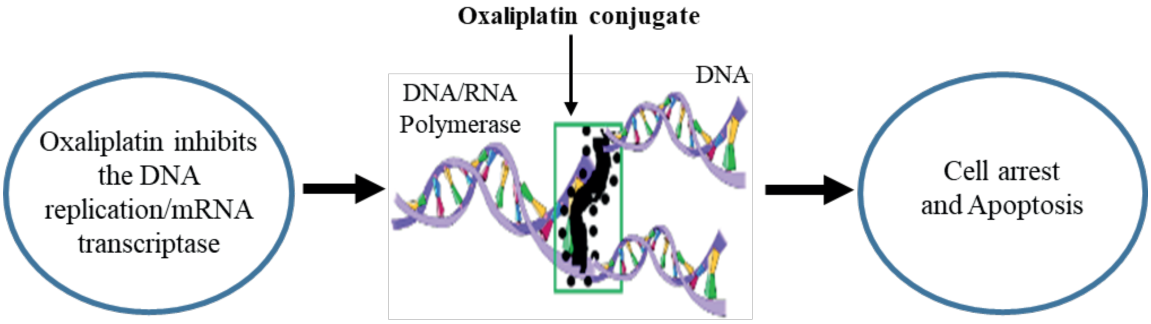
Poster Presentation : **MEDI.P-542**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Intracellular delivery of oxaliplatin conjugate *via* cell penetrating peptide for the treatment of colorectal carcinoma *in vitro* and *in vivo*

Tejinder Singh, **Jungkyun Im**[1,*]

Department of Electronic Materials and Devices Engineering, Soonchunhyang University, Korea
[1]*Soonchunhyang University, Korea*

Abstract: Pt-based drugs are one of the main active agents in colorectal cancer treatment. However, drug resistance and dose-dependent side effects are the main barriers that restrict their clinical applications. As an alternative approach to these issues, we designed and synthesized a cell penetrating peptide (CPP) octaarginine-oxaliplatin conjugate that quickly and successfully delivered oxaliplatin into colon cancer cells. The CPP octaarginine is a well-studied cationic peptide that can play a role as a drug delivery vector. In this work, an octaarginine CPP (RRRRRRRR) was conjugated with oxaliplatin via a specific heterobifunctional linker. The *in vitro* studies showed the conjugate had affinity toward mitochondria inside cells and the MTT assay confirmed that conjugate is active in low micromolar range against colon cancer cells, requiring much lower concentrations than the oxaliplatin alone to reach IC_{50}. More importantly, in the *in vivo* mouse study, the conjugate effectively inhibited tumor growth and showed considerably high antitumor activity, demonstrating the conjugate can perform well *in vivo*. This strategy may offer a new approach for designing oxaliplatin derivatives or prodrugs with remarkable therapeutic capabilities.**References:**1.Abramkin, S., Valiahdi, S.M., Jakupec, M.A., Galanski, M., Metzler-Nolte, N. and Keppler, B.K., 2012. Solid-phase synthesis of oxaliplatin–TAT peptide bioconjugates. Dalton Transactions, 41(10), pp.3001-3005.2.Singh, T., Murthy, A.S., Yang, H.J. and Im, J., 2018. Versatility of cell-penetrating peptides for intracellular delivery of siRNA. Drug delivery, 25(1), pp.1996-2006.3.Singh, T., Kang, D.H., Kim, T.W., Kong, H.J., Ryu, J.S., Jeon, S., Ahn, T.S., Jeong, D., Baek, M.J. and Im, J., 2021. Intracellular Delivery of Oxaliplatin Conjugate via Cell Penetrating Peptide for the Treatment of Colorectal Carcinoma in vitro and in vivo. International Journal of Pharmaceutics, p.120904.4.Scheeff, E.D., Briggs, J.M. and Howell, S.B., 1999. Molecular modeling of the intrastrand guanine-guanine DNA adducts produced by cisplatin and oxaliplatin. Molecular Pharmacology, 56(3), pp.633-643.



Mechanism of Action of Oxaliplatin

Poster Presentation : **MEDI.P-543**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Efficient cannabinoid processing using microwave.

Haneul Ju, Jiyool Kim[1], Pilju Choi[2], Taejung Kim[3], Chung-Min Park[4], Sang Il Jeon[5], Jungyeob Ham[3,*]

Natural Products Research, Gangneung-Wonju National University, Korea
[1]*biological chemistry, university of science and technology, Korea*
[2]*Korea Institute of Science and Technology, Korea*
[3]*Natural Products Research, Korea Institute of Science and Technology, Korea*
[4]*Chemical Advanced Materials, Gangneung-Wonju National University, Korea*
[5]*Department of Chemistry, Gangneung-Wonju National University, Korea*

Cannabis has been widely cultivated in tropical and temperate regions of Central Asia since 12,000 years ago and has been used for centuries as a remedy for asthma and headaches. The main component of cannabis is cannabinoids, and studies on pharmacological mechanisms are very active. Among them, cannabidiol (CBD) has been reported to improve immune function, sedative, antiepileptic, anticonvulsant, and anti-anxiety. Because of these studies, CBD has approved the CBD-based liquid Epidiolex for medicinal use by the FDA. Over the years, a significant number of researchers have used heat treatment on cannabis to obtain CBD. However, in the case of heat treatment of existing cannabis, the manufacturing process is complicated and takes a long time, so it is difficult to standardize the active ingredient, so a new processing method is required. In this poster, we developed a novel processing method and optimized conditions for the selective production of CBD and from cannabinoids through microwave processing.

Poster Presentation : **MEDI.P-544**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Novel Synthesis of *N*,*N*-Dimethylbenzamide via Photo Induced Friedel-Crafts Reaction

Myeonggeuk Kim, Liu-lan Shen[1], Jin-Hyun Jeong*

College of Pharmacy, Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea
[1]*College of Pharmacy, Yonsei University, Korea*

Novel method of photo induced Friedel-Crafts reaction was developed using UV LED and photocatalyst. *N*,*N*-dimethylbenzamide compounds are usually used as active pharmaceutical ingredients. In practically production process traditional Friedel-Crafts reaction often cause environmental pollution and high cost. In this study, we solved this problem using photochemical reaction. Some cases were reported that Friedel-Crafts reaction was completed by photo reaction which was an eco-friendly method and easier to scale-up. Therefore, we conducted a study to directly synthesize *N*,*N*-dimethylbenzamide using photo induced Friedel-Crafts reaction method. As a result, we achieved the *N*,*N*-dimethylbenzamide as major product.

Poster Presentation : **MEDI.P-545**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Investigation of the Neuroinflammation Effects of Diosgenin Derivatives

Young Hun Yoo, Byungsun Jeon*, Sanghee Lee*, Jeong Tae Lee[1]

Research Operations for Brain Science, Korea Institute of Science and Technology, Korea
[1]*Chemistry, Hallym University, Korea*

Diosgenin, a steroidal saponin, is a hydrolyzed product of dioscin produced by the plant family of Dioscoreaceae. Like dioscin, diosgenin, the aglycone of dioscin, shows multiple pharmacological activities such as antitumor, antimicrobial, anti-inflammatory, antioxidative, and tissue-protective properties. Recent studies reported that diosgenin has beneficial in prevention and treatment of neurological diseases such as Alzheimer's disease, Parkinson's disease, and neuroinflammation. Its therapeutic mechanisms have been considered as the mediation of signaling pathways like TLR, NF-κB, JNK, and MAPK. Despite of its various pharmacological activities, however, some drawbacks including the poor solubility in aqueous media and indigent bioavailability obstruct its clinical application. Continuing our previous study, here, we broadened the scope of diosgenin derivatives by the introduction of sulfur or nitrogen at the sugar linking oxygen position. All the synthesized compounds were evaluated by CTG and NO assay, which show cytotoxicity and neuroinflammatory effect. Among them, compound **7** shows relatively good neuroinflammatory effect without leading cell death. To confirm its target and role, we are pursuing through biological studies.

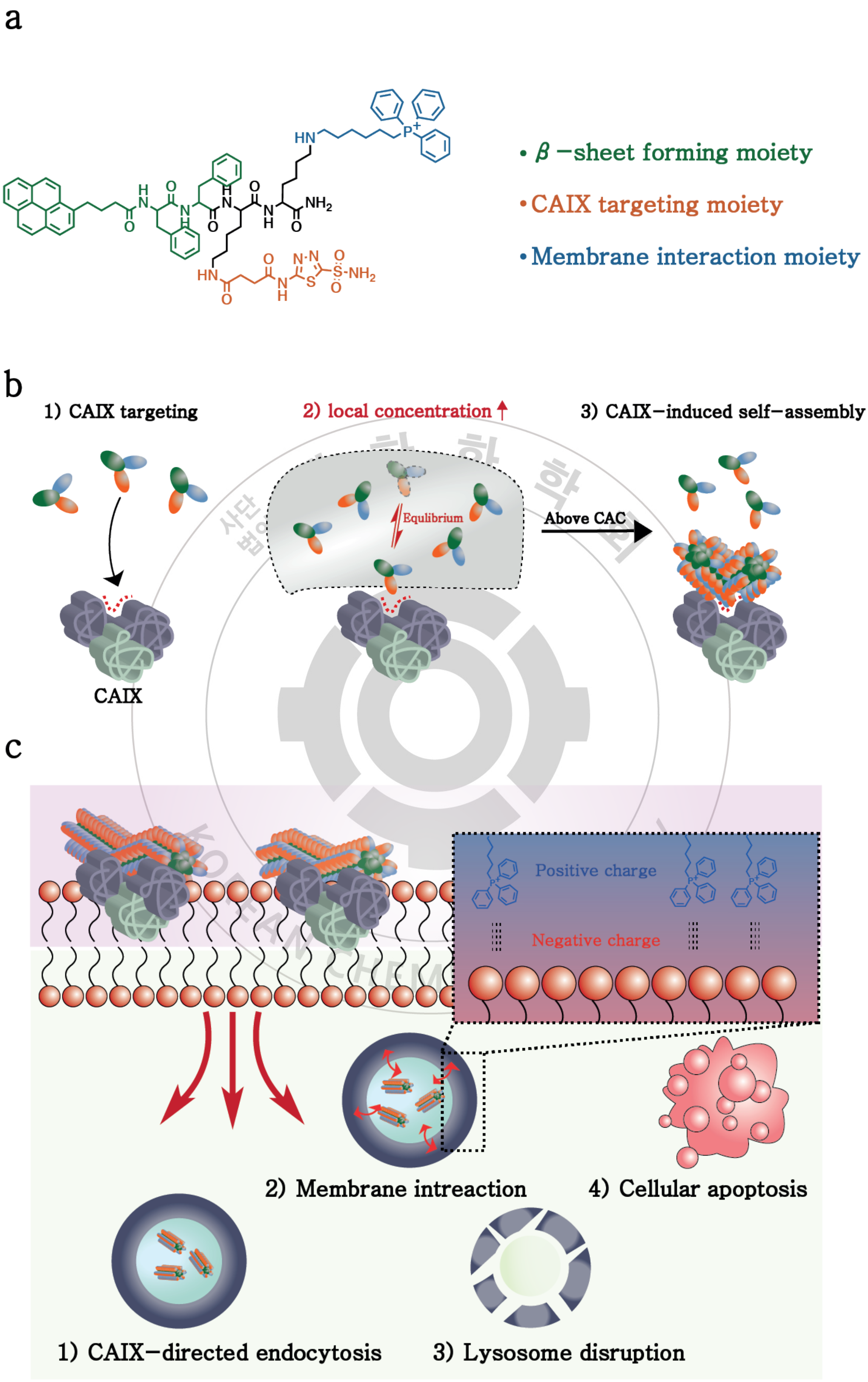
Poster Presentation : **MEDI.P-546**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

CAIX-Targeting Self-Assembly of Peptide Amphiphile in Low Therapeutic Range Inducing Cellular Apoptosis

Dohyun Kim, Ja-Hyoung Ryu*, Sangpil Kim[1], Huyeon Choi

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

Organelle-localization induced supramolecular self-assembly (OLISA) system has been reported for inducing cellular death by destroying an organelle, in which self-assembly structure is formed under spatiotemporal control. It is a novel strategy that could circumvent drug resistance, but overcoming off-targeting effect still re-mains a challenge to solve. Here, we hypothesize that cancer overexpressed enzyme targeting system can be a novel approach to increase the selectivity toward cancer cells, detouring normal cells. We describe an am-phiphilic tetrapeptide, Pep-AT, which contains two different kinds of functional ligands. One is an acetazolamide moiety, which is known for its targeting ability toward carbonic anhydrase IX enzyme (CAIX), and the other is triphenylphosphine (TPP) moiety for increasing organelle membrane interaction. Due to its intrinsic amphiphilic nature, Pep-AT can assemble into nanofiber above critical aggregation concentration. After Pep-AT targets CAIX, a local concentration of Pep-AT around cancer cells increases due to a far-from equilibrium toward CAIX over time, which can endow Pep-AT with driving force to achieve high concentration forming nanofiber structure on a plasma membrane. The nanofiber can be internalized into a lysosome through CAIX-mediated endocytosis. Moreover, a cohesion of the TPP moiety due to self-assembly gives Pep-AT a force to disrupt the organelle membrane. Therefore, Pep-AT can induce the cellular death even in a low therapeutic dose (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1) CAIX targeting
2) local concentration ↑
3) CAIX−induced self−assembly
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Negative charge
2) Membrane intreaction
4) Cellular apoptosis
1) CAIX−directed endocytosis
3) Lysosome disruption

Poster Presentation : **MEDI.P-547**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Design, synthesis and biological evaluation of 2-aminoquinazolin-4-(3H)-one derivatives as potential SARS-CoV-2 and MERS-CoV treatments

Jun Young Lee, Chul Min Park[1,*]

CEVI, Korea Research Institute of Chemical Technology, Korea
[1]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*

Despite the rising threat of fatal coronaviruses, there are no general proven efffective antivirals to treat them. 2-Aminoquinazolin-4-(3H)-one derivatives were newly designed, synthesized, and investigated to show the inhibitory effects on SARS-CoV-2 and MERS-CoV. Among the synthesized derivatives, 7-Chloro-2-((3,5-dichlorophenyl)amino)quinazolin-4(3H)-one and 2-((3,5-dichlorophenyl)amino)-5-hydroxyquinazolin-4(3H)-one showed the most potent anti-SARS-CoV-2 activity (IC50 < 0.25 uM) and anti-MERS-CoV activities (IC50 < 1.1 uM) with no cytotoxicity (CC50 > 25 uM). In addition, both compounds showed acceptable results in metabolic stabilities, hERG binding affinities, CYP inhibitions, and preliminary PK studies.

Poster Presentation : **MEDI.P-548**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Chiral resolution, absolute configuration and biological evaluation of racemic 3,4-dihydroquinazoline derivative

JunSeong Ahn, Gwang Hyun Moon, Seyoung Yang[1], Jiwon Woo[1], Jae Yeol Lee[1,*]

Kyung Hee University, Korea
[1]Department of Chemistry, Kyung Hee University, Korea

The biological properties of different enantiomers often differ greatly due to the stereospecific interactions between target protein and a ligand. One enantiomer is active but the other may be inactive or even toxic. Our group has recently reported that **KCP-10043F** (**OZ-001**) represses the proliferation of human A549 lung cancer cells by caspase-mediated apoptosis via STAT3 inactivation. This compound was a racemate (±)-3,4-dihydroquinazoline derivative with a single chiral center. In order to investigate the difference in biological activities of two enantiomers in a racemic mixture, therefore, chiral resolution of (±)-**KCP-10043F** was performed to achieve the corresponding enantiomers. By the preparation of chiral diastereomers and ^{1}H NMR anisotropy method, the absolute configuration (+)-**KCP-10043F** and (-)-**KCP-10043F** could be assigned as *S* and *R* configuration, respectively. In subsquent biological evaluation, (*R*)-(-)-**KCP-10043F** displayed almost equal cytotoxic activity to (*S*)-(+)-**KCP-10043F** against three cancer cell lines (A549, HT-29 and PANC-1). The possible reason for the equipotency of (*R*)- and (*S*)-**KCP-10043F** in anti-cancer activity was interpreted by molecular docking. The bacterial reverse mutation test (Ames test) for racemate (±)-**KCP-10043F** and its two enantiomers was performed to investigate their latent genotoxicity and all stereoisomers were found to be non-genotoxic against five bacterial strains with /without metabolic activation. Based on these overall results, racemate (±)-**KCP-10043F** (**OZ-001**) could be used for our ongoing preclinical and clinical studies.

Poster Presentation : **MEDI.P-549**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Design and synthesis of *N*-alkyl-1'-(substituted sulfonyl)spiro[chromene-2,4'-piperidin]-6-amine derivatives as anti-inflammatory inhibitors

Lee Hwasung, **Young Dae Gong**[1,*]

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

Design and synthesis of the *N*-alkyl-1'-(substituted sulfonyl)spiro[chromene-2,4'-piperidin]-6-amine based library is presented. Library none with 1-Boc-4-piperidon in the presence of pyrrolidine. The synthesis starts from the pyrrolidine catalyzed cyclization of 1-(2-hydroxy-5-nitrophenyl)ethan-1-one with 1-Boc-4-piperidon according to the previously reported procedure. The resulting tert-butyl 6-nitro-4-oxospiro[chromane-2,4'-piperidine]-1'-carboxylate was then treated with NaBH4 in MeOH and tetrahydrofuran (THF) that led to the conversion of keto group to hydroxyl. The hydroxyl group was tosylated using p-toluenesulfonic acid (pTsOH) in Toluene and tosyl elimination led to the generation of 6-nitrospiro[chromene-2,4'-piperidine] intermediate. Interestingly, the Boc protecting group was removed during the pTsOH treatment. The liberated amine of 6-nitrospiro[chromene-2,4'-piperidine] was then treated with various sulfonyl chlorides in the presence of diisopropylethylamine (DIPEA) for 12 h while heating to yield derivatives. Next, the nitro group was reduced to a primary amine with an iron – ammonium chloride system by refluxing the reaction mixture in EtOH and H2O. The resulting compound was then diversified via reductive amination with various aldehydes affording final *N*-alkyl-1'-(substituted sulfonyl)spiro[chromene-2,4'-piperidin]-6-amine derivatives in good to high yields. The library is expected to be checked for its anti-inflammatory inhibitory activity.

Poster Presentation : **MEDI.P-550**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and evaluation of 2-Aryl-1H-benzo[d]imidazole derivatives as potential microtubule targeting agents

In-ho Song, Gyu Seong Yeom, Su Jeong Park, Satish Balasaheb Nimse*

Institute of Applied Chemistry and Department of Chemistry, Hallym University, Korea

Microtubule targeting agents are the potential drug candidates for anticancer drug discovery. Disrupting the microtubule formation or inhibiting the de-polymerization process by a synthetic molecule can lead to an excellent anticancer drug candidate. Here, we present the 2,5-substituted-1H-benzo[d]imidazole derivatives as potential colchicine, nocodazole binding site targeting agents. About twenty benzimidazole derivatives were synthesized with 82.0% to 94.0% yield using mild reaction conditions. The synthesized compounds showed moderate to excellent anticancer activity established in three cell lines, including Hela cells, A549 cells, and MRC-5 cells. The compounds B15, B16, B19, and B20 are the potential candidates with the IC50 values 100 µM. In the MTT assay, compounds B15, B16, B19, and B20 showed excellent antiproliferation activity indicated by IC50 values in the range of 5.3 ± 0.21 to 18.1 ± 0.32 µM in HeLa, A549 cell line study. The predicted ADME properties and drug-likeness properties of B15, B16, B19, and B20 indicate that these compounds can be used as lead compounds for further study to develop excellent microtubule targeting agents.

Poster Presentation : **MEDI.P-551**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Antiviral effects of triazinoindole derivative that inhibits the interaction between ACE2 receptor and spike protein in SARS-CoV-2 infection

Dongwan Kang, Soong-Hyun Kim, Jee-Young Lee[1], Jiyoun Lim[2], Ha-Yeon Lee[3], Sejin Jung[*]

Medicinal chemistry department, Daegu-Gyeongbuk Medical Innovation Foundation, Korea
[1] *Structure-based Drug Discovery department, Daegu-Gyeongbuk Medical Innovation Foundation, Korea*
[2] *Toxicity and Safety evaluation department, Daegu-Gyeongbuk Medical Innovation Foundation, Korea*
[3] *Safety Assessment department, Daegu-Gyeongbuk Medical Innovation Foundation, Korea*

The current global pandemic COVID-19 is the severe acute respiratory syndrome caused by SARS-CoV-2 virus but effective therapeutics against COVID-19 are still unavailable except for the broad spectrum antivirals such as remdesivir, favipiravir and chloroquine. ACE2 (angiotensin-converting enzyme 2) is a type 1 transmembrane metallocarboxypeptidase and acts as a host receptor for virus entry into the human cells. Spike protein of SARS-CoV-2 contains RBD (receptor binding domain) that specifically recognizes ACE2 as its receptor and is proteolytically activated by human proteases to achieve its function. Therefore, blocking the interaction between ACE2 receptor and spike protein is a potential therapeutic target to prevent SARS-CoV-2 infection. We have discovered compound 15 as a lead compound to develop COVID-19 antiviral agent, obtained from *in silico* library screening combined with ACE2-RBD binding assay and *in vitro* antiviral assay. The results showed that compound 15 prevents SARS-CoV-2 infection in Vero cell with an IC_{50} value of 0.65uM, which is more potent than reference drugs like remdesivir, lopinavir and chloroquine in our assay system. In addition, ADME properties indicated that compound 15 is fairly stable in plasma and liver microsomes and has no inhibition on cytochrome P450 enzymes.

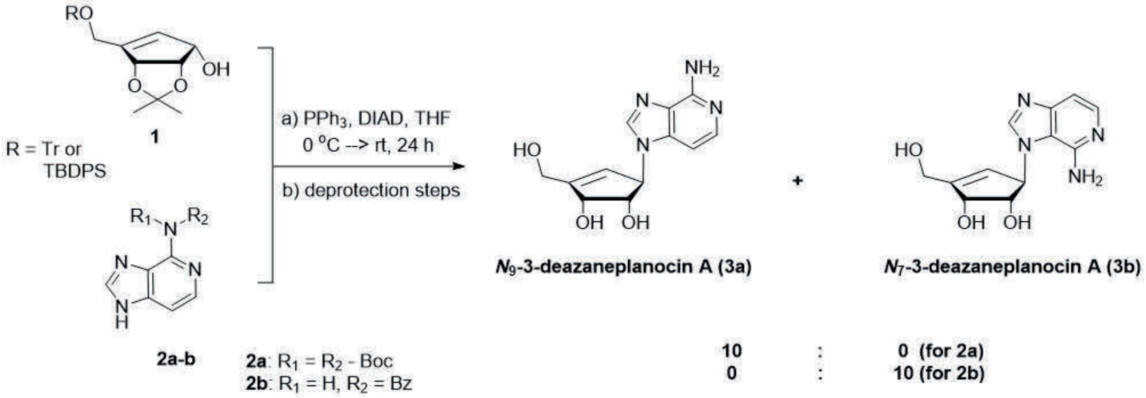
Poster Presentation : **MEDI.P-552**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Regioselective Synthesis of 3-Deazaneplanocin A Derivatives and their Antiviral Acitivity against Infleunza A Virus

SeMyeong Choi, Yeon Jin An, Yeeun Nam, EunRang Choi, Eunwoo Seo, Jong Hyun Cho*

Department of Health Sciences, Dong-A University, Korea

An efficiently regioselective synthesis of N_7- and N_9-3-deazaneplanocin A have been developed by using Mitsunobu reaction[1] of N^6 -protected 3-deazpurine derivatives with a cyclopentenol moiety (**1**). The coupling reaction of **1** with N^6 -bisBoc-3-deazapurine (**2a**) mainly provided N_9-3-deazaneplanocin A derivative in the presence of DIAD, Ph_3P in THF. Unexpectedly, the Mitsunobu reaction of **1** with N^6 -Bz-3-deazapurine (**2b**) afforded only N_7-3-deazaneplanocin A in excellent yield without detection of the N_9-isomer. After removal of all protection groups, N_7- and N_9-3-deazaneplanocin A derivatives were obtained as their corresponding N_7- and N_9-3-deazaneplanocin As (**3a**-**b**). In vitro assay, N_9-3-deazaneplanocin A (**3a**) showed potency against Flu A (H1N1) (EC50 25 μM), whereas N_7-3-deazaneplanocin A (**3b**) exhibited mild activity against Flu A (H5N1) (EC50 29.0 μM), Flu B (EC50 8.0 μM)[2,3]. The novel compound (**4a**) exhibited potent activity against Flu A (H1N1) (EC50 7.6 μM).



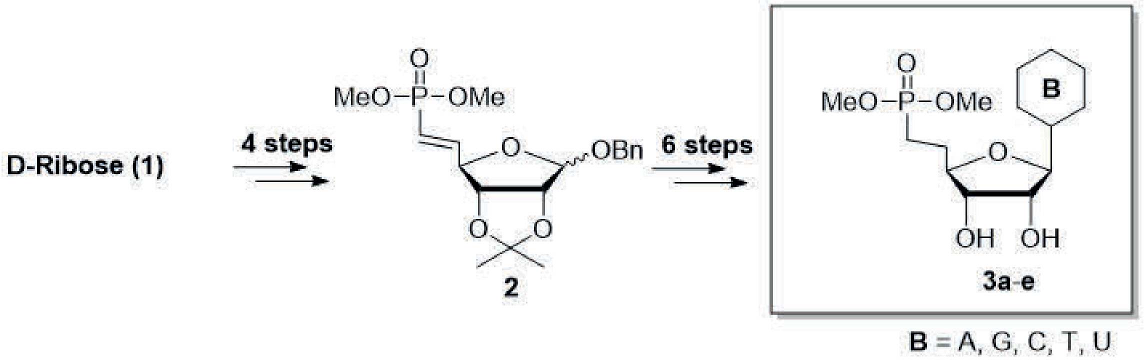
Poster Presentation : **MEDI.P-553**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Efficient Synthesis of D-Nucleoside Phosphonate Prodrugs using Cross Metathesis

Yeeun Nam, SeMyeong Choi, Choi EunRang, Eunwoo Seo, Yeon Jin An, Jong Hyun Cho*

Health science , Dong-A University, Korea

The phosphonate D-ribonucleotide prodrugs were efficiently synthesized by using the cross metathesis (CM) reaction.[1] The key intermediate, D-ribolactol phosphonate, was prepared from D-ribose in 4 steps.[2] The oxidation of 5-OH with IBX and then wittig reaction after reaction of D-ribose with acetone followed by protection of 1-OH with Benzyl group afforded protected D-ribolactol in quantitative yield. Following this, the CM reaction of D-ribolactol with terminal olefin derivatives using a H-G catalyst II[3] provided their corresponding phosphonates. Subsequently, the treatment of D-ribolactol phosphonate (**2**) with HCl/MeOH, BzCl, acylation, and hydrogenation gave 1-*O*-Ac-2,3-*O*-diBz-D-ribolactol phosphonate. The coupling reaction of the phosphonate with the persilylated natural bases (A, G, C, T, U) using $SnCl_4$, followed by deprotection of Bz gave D-ribonucleotide analogs (**3a**-**e**) in good yield, respectively. [4]



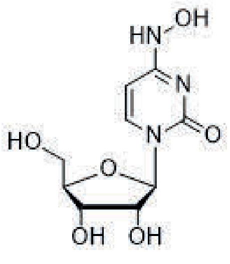
Poster Presentation : **MEDI.P-554**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

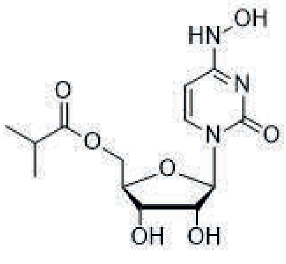
Synthesis and evaluation of *β*-D-*N*^{4}-hydroxycytidine (NHC) prodrugs against SARS-CoV-2 in vitro

Yeon Jin An, SeMyeong Choi, Yeeun Nam, Eunwoo Seo, EunRang Choi, Jong Hyun Cho[1,*]

Health science, Dong-A University, Korea
[1]*Medicinal Biotechnology, Dong-A University, Korea*

As the pyrimidine nucleoside, *β*-D-*N*^{4}-hydroxycytidine (NHC, EIDD-1931) analogs have exhibited a broad spectrum of antiviral activity against anti-RNA viruses such as SARS-CoV, MERS-CoV, norovirus, chikungunya virus, Yellow FV, WNV, JEV, and Zika virus.[1] We herein present synthesis of several NHC derivatives as modification of MK-4482 (EIDD-2801)[2,3], which is currently in phase II/III clinical trials for global pandemic SARS-Cov-2 infection.[4] Additionally, we wish to report the NHC prodrug (CD-I-100) showed significant antiviral activity (EC50 1.20 μM) against SARS-CoV-2 in vitro.


NHC(EIDD-1931)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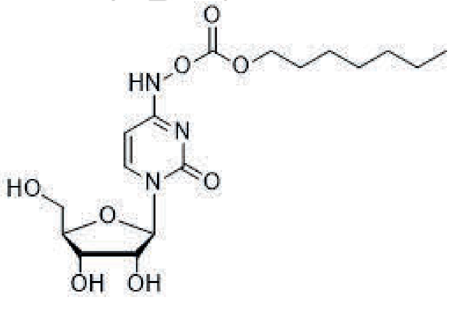

CD-I-100

Poster Presentation : **MEDI.P-555**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Evaluation of Acyclic five-membered base nucleoside derivatives

EunRang Choi, Eunwoo Seo, Yeeun Nam, SeMyeong Choi, Yeon Jin An, Jong Hyun Cho*

Health science, Dong-A University, Korea

Based on the broad spectrum of antiviral activity of the Ribavirin, it was necessary to synthesize its nucleoside analogs for targeting a specific RNA virus. Novel five-membered base nucleoside analogs were successfully synthesized from (**1**-**53**) acyclic side chains by using Mitsunobu reaction to find antiviral compounds against RNA virus. As Ribavirin, compounds (**1**-**53**) were synthesized from commercially available pyrazole, imidazole, triazole by using Mitsunobu reaction. Coupling reaction of acyclic sugar moieties (**1a**-**e**) with five-membered heterocyclic analogs, followed by removal of protecting group(s) provided their corresponding nucleoside ester analogs (**1**-**20**) in moderate to good yields. (Fig 1) The treatment of nucleoside ester analogs with ammonia or hydroxy amine[1,2] afforded their corresponding nucleoside analogs (**21**-**53**) in good yields. Among synthetic compounds, imidazole analog showed activity (EC_{50} 25 μM) against Flu A (H1N1). (Fig 2)

Figure 1.

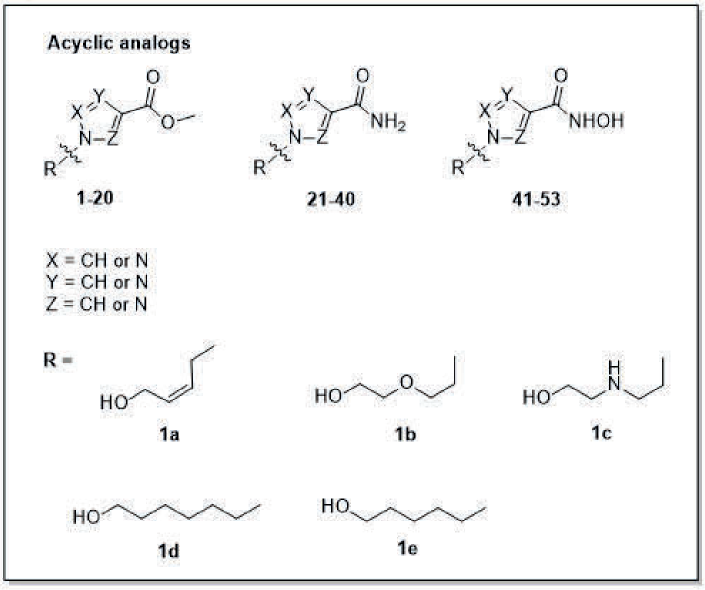
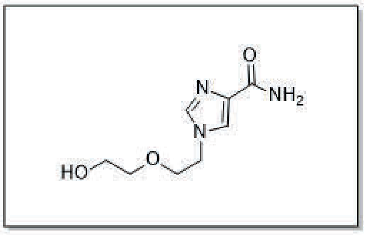


Figure 2.



Poster Presentation : **MEDI.P-556**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Development of new target protein catalyst compounds as a novel class of H2O2 scavenger for treatment of Alzheimer's Disease

Elijah Lee, Ki Duk Park[1,*]

Convergence Research Center for Diagnosis, Treatment and Care System of Dementia, Korea Institute of Science and Technology, United States
[1]*Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

Alzheimer's disease (AD) is the most common form of dementia and is a progressive neurodegenerative disease characterized by memory loss. In the AD brain, reactive oxygen species (ROS) levels are significantly higher than that of healthy aging brain. Hydrogen peroxide (H2O2) is a representative ROS that causes oxidative stress and is a product of many different metabolic pathways in AD. We recently investigated the mechanism of action of the drug AAD-2004, which is effective in scavenging H2O2 in neurodegenerative disease mouse model. In this study, we aim to optimize the efficacy and drug-like properties of AAD-2004 to develop a novel H2O2 target candidate for treatment of AD. We synthesized 33 novel compounds and evaluated the H2O2 scavenging activity using an optimized in vitro assay system. Among them, KDS12025 exhibited five times the efficacy of AAD-2004 (EC50: 0.199 μM to 0.99 μM, respectively) and also showed favorable microsomal stability (57.6% in human during 30 min to

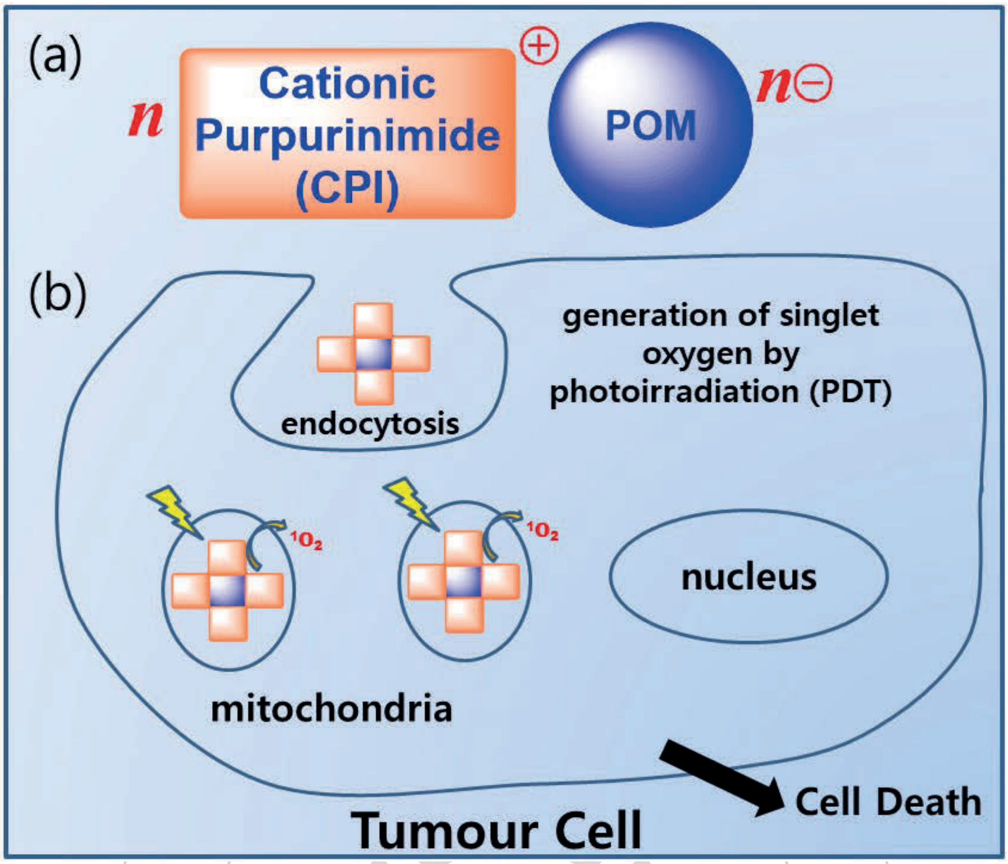
Poster Presentation : **MEDI.P-557**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Mitochondrial Targeting Cationic Purpurinimide–Polyoxometalate Supramolecular Complexes for Enhanced Photodynamic Therapy with Reduced Dark Toxicity

Il Yoon

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

Polyoxometalates (POMs), that are well-defined metal-oxygen cluster anions, are functional molecules extensively used in various research applications. The synthesis of neutral purpurinimides, followed by conversion to cationic purpurinimides (CPIs), formed CPI–POM supramolecular complexes via electrostatic interactions between each CPI and the polyanionic POM. The cellular uptake of purpurinimides, CPIs, and their CPI–POMs in A549 and HeLa cell lines was confirmed by confocal laser scanning microscopy. CPIs showed concentration-dependent dark cytotoxicity; however, CPI–POMs exhibited reduced low dark cytotoxicity. After photoirradiation, CPIs and CPI–POMs revealed enhanced photodynamic therapy (PDT) compared to free purpurinimides against A549 and HeLa cells. The CPIs exhibit low cell viability by incorporating their PDT effect with intrinsic dark cytotoxicity; however, the CPI–POMs exhibited a POM delivery effect-based enhanced PDT activity in the supramolecular complex system with low dark cytotoxicity. In particular, the clicked CPI–POM revealed two times higher PDT activity compared with the clicked free CPI, due to the good delivery effect of POM.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n
Cationic Purpurinimide (CPI)
+
POM
n−
(b)
endocytosis
generation of singlet oxygen by photoirradiation (PDT)
$^1O_2$
$^1O_2$
nucleus
mitochondria
Cell Death
Tumour Cell

Poster Presentation : **MEDI.P-558**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Identification of Highly Selective Type II Kinase Inhibitors with Chiral Peptidomimetic Tails

Jaeeun Jung, HeeJin Jeong, Duck-Hyung Lee[1], Taebo Sim[2,*], Seojung Han[*]

Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea
[1]*Department of Chemistry, Sogang University, Korea*
[2]*Severance Biomedical Science, Yonsei University, Korea*

Identification of extremely selective type II kinase inhibitors is described. Two different types of chiral peptidomimetic scaffolds were introduced on the tail region of GNF-7, which is a non-selective type II kinase inhibitor, to enhance selectivity. Kinome-wide selectivity profiling analysis showed that type II kinase inhibitor **7a** potently (IC_{50} of 23.0 nM) inhibited Lck kinase with exceptional selectivity. It was found that **7a** and its derivatives possessed high selectivity for Lck over even structurally conserved all Src family kinases. The superior selectivity of **7a** could be explained in part by computational analysis with MD simulation and WaterMap application. Moreover, we observed that both **7a** and **7f** are capable of inhibiting phosphorylation of Lck in Jurkat cells. This study provides a novel insight into the design of selective type II kinase inhibitors by adopting chiral peptidomimetic moieties on the tail region.

Poster Presentation : **MEDI.P-559**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Purpurinimide Derivative-Graphene Oxide Nanoparticles for Enhanced Photodynamic Therapy

Hyerim Kim, Il Yoon[1,*]

Inje University, Korea
[1]*Center for Nano Manufacturing and Department of Nanoscience and Engineering, Inje University, Korea*

Graphene oxide (GO) is used for biomedical applications, such as drug delivery, biological imaging, and phototherapy. Photodynamic therapy (PDT) is a non-invasive and patient-specific cancer treatment using a photosensitizer (PS), light and oxygen. We synthesized purpurinimide derivative as a long wavelength absorbing PS and combined with GO as a good delivery vehicle as well as photothermal therapy (PTT) to generate purpurinimide derivative-GO nanoparticles via non-covalent bonds for enhanced PDT/PTT combination cancer therapy.

Poster Presentation : **MEDI.P-560**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Highly potent and selective PPARδ agonist reverses memory deficits and can be novel therapeutic agent in Alzheimer's disease

Hyeon Jeong Kim, Jungwook Chin[1,*], Ki Duk Park[*]

Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea
[1]*New Drug Development Center, Daegu-Gyeongbuk Medical Innovation Foundation, Korea*

Alzheimer's disease (AD) is a progressive neurodegenerative disease accompanied by neurotoxicity, excessive inflammation, and subsequent cognitive impairment. Peroxisome proliferator-activated receptor (PPAR) δ plays a vital role in fatty acid metabolism as a lipid sensor and regulates inflammatory responses in the central nervous system (CNS). Here, we investigated anti-inflammatory effects of a novel PPARδ agonist (5a) and the therapeutic effects on AD-like pathology. 5a suppressed inflammatory responses in activated BV-2 microglial cell and mouse model of AD. Oral administration of 5a ameliorated glial activation and deposition of amyloid plaques, leading to improved learning and memory in APP/PS1 mice. Our findings suggest that PPARδ-mediated anti-inflammatory effects may be beneficial in AD.

Poster Presentation : **MEDI.P-561**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of Novel Sphingosine-1-Phosphate-1 (S1P$_1$) Receptor Agonists for the Treatment of Multiple Sclerosis

Ki Duk Park[*], **Yoowon Kim**[1]

Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea
[1]*Korea Institute of Science and Technology, Korea*

The sphingosine-1-phosphate-1 (S1P$_1$) receptor agonists have great potential to treat multiple sclerosis (MS) because they can inhibit lymphocyte egress through receptor internalization. We designed and synthesized azetidine, pyrrolidine, and piperidine derivatives to discover a novel S1P$_1$ agonist for MS treatment. Azetidine derivatives were determined to have excellent in vitro efficacy and drug-like properties. Among them, compound **21l** was found to have superior drug-like properties as well as excellent in vitro efficacies (EC$_{50}$ = 7.03 nM in β-arrestin recruitment; EC$_{50}$ = 11.8 nM in internalization). We also confirmed that **21l** effectively inhibited lymphocyte egress in the peripheral lymphocyte count (PLC) test and significantly improved the clinical score in the experimental autoimmune encephalitis (EAE) MS mouse model.

Poster Presentation : **MEDI.P-562**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of a potent and novel small molecular ENPP1 inhibitor

HeeJin Jeong, Chan Sun Park[1], Hyo Jae Yoon, Duck-Hyung Lee[2], Sanghee Lee[3,*], Seojung Han[4,*]

Department of Chemistry, Korea University, Korea
[1]*TXINNO Bioscience INC., Korea*
[2]*Department of Chemistry, Sogang University, Korea*
[3]*Neuromedicin department, Korea Institute of Science and Technology, Korea*
[4]*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

The innate immune Stimulator of Interferon Genes (STING) pathway is activated by cyclic GMP-AMP (cGAMP) in response to cytosolic foreign double-stranded DNA from cancers. An ectonucleotide pyrophosphatase/phosphodiesterase 1 (ENPP1) negatively regulates the STING pathway by hydrolyzing cGAMP. In an effort to discover novel scaffolds of non-nucleotide-derived ENPP1 inhibitors, we designed pyrrolopyrimidine and pyrrolopyridine derivatives and performed structure-activity relationship (SAR) study. We found **10p** possessed high potency (IC_{50} = 19.0 nM), and activated STING pathway in a concentration dependent manner. Also, cytokines such as IFN-β and IP-10 were induced by **10p** in a concentration dependent manner.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **MEDI.P-563**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Synthetic Study of Novel Drug-like Thieno pyrazine Derivatives as DNA Base Biomimetics

Dana Kim, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

Cancer is a serious disease that is the leading cause of death in Korea. However, most anticancer drugs have side effects such as toxicity from anticancer drugs that can damage normal cells. Therefore, it is still required to develop an anticancer drug that can overcome the side effects of the current anticancer drugs. In connection with such efforts, researchers have conducted a prior investigation and noticed that thieno pyrazine derivatives have low toxicity while showing excellent anticancer activity. In this respect, we were interested in the synthesis of thieno pyrazine derivatives. First, the reaction of 5-bromo-6-chloropyrazine-2-amine and trimethylsilylacetylene would provide valuable 6-chloro-5-((trimethylsilyl)ethynyl)pyrazin-2-amine intermediate via Sonogashira reaction. Next, the 6-chloro-5-((trimethylsilyl)ethynyl)pyrazin-2-amine intermediate could undergo cyclization with $Na_2S{\cdot}5H_2O$ further functionalization using various electrophiles like alkyl halides, acid chlorides to give a range number of theino pyrazine derivatives.

Poster Presentation : **MEDI.P-564**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

2-Thioxothiazolidin-4-one Analogs as Pan-PIM Kinase Inhibitors

Seungik Jeong, Jinho Lee[*], Victor Sukbong Hong[*], Hyeonseong Choo[1]

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

Proto-oncogenic proviral integration site for Moloney murine leukemia virus (PIM) kinases are involved in the regulation of several cellular processes. PIM kinases are considered as promising targets for cancer treatments because they play a major role in many cancer-related pathways, such as survival, apoptosis, proliferation, and migration. Here, a novel analogous of 2-thioxothiazolidin-4-one were synthesized and evaluated as potent pan-PIM kinase inhibitors. Optimization and structure-activity relationship studies yielded inhibitors with single-digit nanomolar IC50 values against all three PIM kinases. Compound 17 showed high selectivity over 14 other kinases and inhibited the growth of leukemia cell lines (Molm-16, EC50 = 14 nM). It also modulated the expression of pBAD and p4EBP1 in a dose-dependent manner.

Poster Presentation : **MEDI.P-565**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Effective Photodynamic Therapy Overcoming Hypoxia by Protein Coated Metal-Organic-Framework

Youjung Sim, Huyeon Choi, Myoung Soo Lah*, Ja-Hyoung Ryu*

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

Photodynamic Therapy (PDT) is a form of a phototherapy inducing cell death using light, oxygen and Photosensitizer (PS) which is generating ROS. These ROS interact with cellular components including lipids, amino acid and nucleic acids, and lead to the cell dysfunction. However, as a tumor grows, it rapidly outgrows its blood supply, leaving portions of the tumor where the oxygen concentration is significantly lower than in healthy tissues. For this reason, even effective photosensitizers cannot be working efficiently as much as expected. Therefore, if we overcome this hypoxia environment of tumor, photodynamic therapy can be more effective way forward. In our research, we conjugate the enzyme catalase (CAT) to surface of biocompatible nanocarrier MOF808. Catalase catalyzes the decomposition of hydrogen peroxide (H2O2) to water (H2O) and oxygen (O2). The generated oxygen can relieve the Hypoxia condition in tumor. Enriched oxygen further increases the PDT effect, enabling effective ROS generation. Also, immobilized enzyme is more stable than the free form of the enzyme enhancing the recyclability of enzymes and minimizing enzyme contamination.

Poster Presentation : **MEDI.P-566**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Inhibition of ACE2-Spike interaction by an ACE2 allosteric binder suppresses SARS-CoV-2 entry

Kiyoung Jeong, Jonghoon Kim[1], Seung Bum Park*

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

The sudden emergence and rapid spread of severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) have posed a severe global public health emergency. The most serious problem is that the variants of SARS-CoV-2 obstruct the development of effective therapeutics and vaccines in the middle of the coronavirus disease 2019 (COVID-19) pandemic. Here, we discovered a novel small molecule that inhibits the interaction between receptor binding domain (RBD) of the spike protein of SARS-CoV-2 and human cell receptor ACE2 by modulating ACE2 without damaging its enzymatic activity necessary for normal physiological functions. Furthermore, the discovered compounds suppress the viral infection in cultured cells by hampering the entry of ancestral and SARS-CoV-2 variants. Thus, our discovery could be used as a novel therapeutic strategy to overcome the current COVID-19 pandemic by inhibiting SARS-CoV-2 entrance.

Poster Presentation : **MEDI.P-567**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

N-(2,7-Dimethyl-2-alkyl-2H-chromen-6-yl)sulfonamide derivatives as selective serotonin 5-HT6 receptor antagonists: design, synthesis, and biological evaluation

Young Dae Gong[*], **Young-Chang Kim**

Department of Chemistry, Dongguk University, Korea

Serotonin 5-HT6 receptor, which is predominantly expressed in the central nervous system, is a valuable therapeutic target. Serotonin 5-HT6 receptor antagonists have potential for the treatment of various diseases that include psychotic disorders, dementia, depression, and obesity. In this study, we designed and synthesized the N-(2,7-dimethyl-2-alkyl-2H-chromen-6-yl)sulfonamide-based library as a potential serotonin 5-HT6 receptor antagonist. The library was subjected to a series of binding affinity tests to identify the lead compound, and check the selectivity of test compounds towards the 5-HT6 receptor. Accordingly, compound N-(2,2,7-trimethyl-2H-chromen-6-yl)naphthalene-2-sulfonamide was identified as the most active compound, with IC50 = 87 nM. The binding affinity of 95.3% of N-(2,2,7-trimethyl-2H-chromen-6-yl)naphthalene-2-sulfonamide (10 M) with the 5-HT6 receptor among other serotonin 5-HT1a, 5-HT2a, 5-HT2c, and 5-HT7, and dopamine receptors D1, D2, D3, and D4, demonstrated the high selectivity of N-(2,2,7-trimethyl-2H-chromen-6-yl)naphthalene-2-sulfonamide towards the 5-HT6 receptor.

Poster Presentation : **MEDI.P-568**

Medicinal Chemistry

Exhibition Hall 1 FRI 11:00~12:30

A Comparison Study of Photothermal Effect Between Gold Nanoparticles and Ultrasmall Copper Nanoparticles under NIR Stimuli

Hyojin Cho, Sang Eun Hong, Mi Jin Park, Kuk Ro Yoon*

Department of Chemistry, Hannam University, Korea

Metal nanoparticles with diverse material properties have special physicochemical characteristics and opportunities for optics, novel biological and biomedical applications. Particularly, the unique photochemical profiles of nanomaterials were researched. Synthesis of highly stable dispersions of copper and gold nanoparticles in aqueous solution were using a cost-effective and green method. In this study, ultrasmall sized Cu nanoparticles with diameters of under 5 nm were prepared through L-ascorbic acid reducing agent also, gold nanoparticles. Which was confirmed the unique photothermal effect under near-infrared ray (NIR) stimuli. Also, that's nanoparticles were characterized by UV-vis (Ultraviolet-visible spectroscopy), FE-TEM (Field-emission Transmission Electron Microscope), DLS (Dynamic Light Scattering), and photothermal performance.

Poster Presentation : **MEDI.P-569**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Development of Bioorthogonal Linkers for Surface Modification of Silica Nanoparticles

<u>Jeunghwan Kim</u>, Jaewoon Lee, InCheol Heo[1], Won Cheol Yoo[2], Sun-Joon Min[3,*]

Department of 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

Silica nanoparticles (SNPs) have attracted attention in recent years as versatile carriers for drug delivery due to their structural properties such as controllable particle size, colloidal stability, and high surface area. They can be functionalized by introducing organic molecules to their surface through a covalent bond, which provides high biocompatibility as well as their cargo capability. In general, the reactions between alkoxysilanes and hydroxyl groups of SNPs have been used as SNPs surface-grafting methods. Although the alkoxysilanes are widely used for surface modification, it is difficult to synthesize modified alkoxysilanes because they are easily decomposed during functional group transformation. Furthermore, only one functional molecule can be installed on the surface of SNP via covalent bond formation.In this study, we described development of SNPs containing dual linkers that can operate in a bioorthogonal fashion. We designed and synthesized two kinds of allylsilane reagents containing strained alkenes and maleimides respectively as crucial components. We successfully introduced both allylsilanes to SNPs using Lewis acid-promoted siloxane formation, which were finally applied to labeling of fluorescent dyes and isotopes through bioorthogonal cycloaddition and conjugate addition.

Poster Presentation : **MEDI.P-570**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

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

Kyungjin Jung, Jungwook Chin*

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

Psiguadial B (8), and its fluoro- (8a), chloro- (8b), and bromo- (8c) derivatives were synthesized using a sodium acetate-catalyzed single step coupling of three components: β-caryophyllene (5), diformylphloroglucinol (11), and benzaldehyde (12). These compounds efficiently and dose-dependently decreased H2O2-induced cell death, a quantitative marker of cell death, in primary cultures of mouse cortical neurons. Psiguadial B also decreased neuronal death and accumulation of ROS induced by FeCl2 in cortical cultures. The in vitro effects of these compounds in lipopolysaccharide (LPS)-induced expression of nitric oxide (NO), and TNF-α and IL-6 by suppressing the NF-κB pathway in immune cells demonstrated their antioxidative and anti-inflammatory activity. The present findings warrant further research on the development of psiguadial B-based neuroprotective agents for the treatment of neurodegenerative diseases, acute brain injuries and immunological disorders.

Poster Presentation : **MEDI.P-571**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Antioxidative and Tyrosinase Inhibitory Activities of mixed Ishige okamurae extract and Wolfiporia extensa extract

Seonyeong Ahn*, **Mingyeong Kim[1,*]**, **Byong Wook Choi[2]**, **Bong Ho Lee[1,*]**

Chemical & Biological engineering, Hanbat National University, Korea
[1]*Department of Chemical and Biological Engineering, Hanbat National University, Korea*
[2]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

It is known that MeOH extract of Wolfiporia extensa contains taxifolin, taxifolin-3-O-glucoside, and other flavonoids. It also has pangamic acid, polypotenic acid A, triterpenoids, lecithin, and other secondary metabolites. It does not have notable toxicities, thus it is suitable for commercial applications.The authors found that the BuOH extract of a brown seaweed, Ishige okamurae has strong antioxidative, elastase and collagenase inhibitory activities. Thus, the authors decided to measure the antioxidative and enzyme inhibitory activities of the mixture of EtOH extracts of two samples to know a possible application. We obtained natural Wolfiporia extensa collected in Youngchun and Ishige okamurae collected offshore of Jeju and prepared EtOH extract for each sample. The extraction yield depends on a water content. It is increased as the water content is increased. The mixture of these two extracts at different ratio showed a similar DPPH scavenging activity to each extract implying the radical scavenging activity of the two is very close. These extracts also showed moderate tyrosinase inhibitory activity, 33% inhibition at 0.1 mg/mL.

Poster Presentation : **MEDI.P-572**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Selenocyanation of Aryl Methyl Ketones for novel selenazolamine compounds

Il Park, Liu-lan Shen[1], Jin-Hyun Jeong[*]

College of Pharmacy, Yonsei Institute of Pharmaceutical Sciences, Yonsei University, Korea
[1]*College of Pharmacy, Yonsei University, Korea*

Organoselenium compounds become active ingredients in the pharmaceutical field. Here, we designed novel selenazolamine compounds for biological activity like anti-tumor, anti-inflammatory, and anti-aging.We studied and introduced Selenocyanation of Aryl Methyl Ketones ad efficient synthetic route, direct and one-pot reaction using selenium dioxide and malononitrile. under moderate conditions could give meaningful yield.

Poster Presentation : **MEDI.P-573**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Design and Synthesis of Novel MAO-B PET Probe Candidate for Diagnosis of Reactive Astrocyte

Byungeun Kim, Ki Duk Park[1,*]

Bio-Medical Science & Technology, University of Science and Technology, Korea
[1]*Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

Astrogliosis occurs by abnormal CNS pathological conditions. Especially in various neurodegenerative conditions, astrogliosis appears frequently. A recent study found that these reactive astrocytes generate GABA through upregulated MAO-B enzyme, causing memory impairment in Alzheimer’s disease. As a follow-up study of these previous discoveries, our group have synthesized selective, reversible and novel MAO-B inhibitor, KDS2010. MAO-B, not only as a therapeutic target of neurodegenerative diseases, but also could be a promising target for diagnosis of reactive astrocytes. It was found that MAO-B is overexpressed in the brain of patients with neurodegenerative disease, and accordingly, there has been development of PET tracers targeting MAO-B. But, previously developed tracers are not reversible or having short half-life of [^{11}C]. So I tried to synthesize novel fluorinated MAO-B PET probe candidate based on KDS2010 structure and developed Compound **6a**. **6a** has exhibited potent inhibition effect on MAO-B (IC50 = 7 nM) with favorable microsomal stability data and CYP inhibition safety. PK study also showed probability of PET tracer. Finally, in order to increase the possibility of clinical application as a PET trace, one-pot synthesis procedure and HPLC purification method were optimized.

Poster Presentation : **MEDI.P-574**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and evaluation of a novel series of vinyl sulfone derivatives from Veda-1209 as promising Nrf2 activators

Rium Kim, Ki Duk Park[1,*]

Convergence Research Center for Dementia, University of Science & Technology, Korea
[1]*Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

The Nrf2 signaling is the main pathway responsible for cellular defense system against oxidative or electrophilic stress. Nrf2 plays a vital role in anti-inflammatory responses as well as antioxidant defenses by mediating the expression of various antioxidant enzyme genes and pro-inflammatory cytokines. Several studies have reported that chalcone consisting of α,β-unsaturated carbonyl system exhibit several biological activities including anticancer, antioxidant, antibacterial and anti-inflammatory properties. Veda-1209, a chalcone derivative, is Nrf2 activator currently undergoing preclinical testing for the treatment of various diseases.In this work, a series of novel Veda-1209 derivatives were synthesized by substituting vinyl sulfone and screened for their Nrf2 activating efficacy, antioxidant and anti-inflammatory effects in vitro. Among the synthesized compounds, a lead compound (**1**) exhibited superior Nrf2 activation and drug-like properties compared to Veda-1209 (Nrf2 activation EC50: Veda-1209 = 625 nM vs compound **1** = 58 nM). Furthermore, compound **1** induced the expression of the Nrf2-dependent enzymes at both mRNA and protein levels and suppressed the induction of pro-inflammatory cytokines and enzymes. In conclusion, compound **1** represents a novel Nrf2 inducers with potential to act as antioxidant and anti-inflammatory agents.

Poster Presentation : **MEDI.P-575**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of harmala alkaloid analogs as anticancer agents

<u>Yunha Choi</u>, Vineetkumar Bapusaheb Patil[1], Seong Hwan Kim[2], Pilho Kim[3,*]

Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea
[1]*Medicinal Chemistry, University of Science & Technology / KRICT, Korea*
[2]*Drug Discovery Platform Research Center, Korea Research Institute of Chemical Technology, Korea*
[3]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Harmala alkaloids (HA), such as harmine, harmaline, and harmalol, are known to be monoamine oxidase inhibitors and exhibit anticancer activities. The tricyclic core structure of HA is composed of β-carboline, 9*H*-pyrido[3,4-*b*]indole. There are numerous biological activities and synthetic methods known to date. Recently, we performed a high-throughput screening of HA analog library against several cancer cell lines and discovered hit compounds. Based on what we developed for the synthesis of tetrahydroisoquinoline analogs, we will report synthetic pathways to prepare HA analogs, and their anticancer activities. Moreover, structure-activity relationships and anticancer mechanism of the compounds prepared will be discussed.

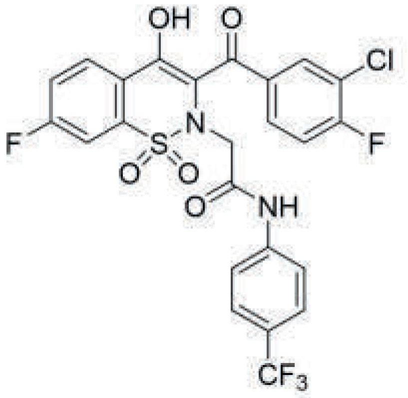
Poster Presentation : **MEDI.P-576**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of cyclic sulfonamide derivatives as potent inhibitors of SARS-CoV-2

Chul Min Park[*], Young Sup Shin[1]

Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea
[1]*Center for convergent research of emerging virus infection, Korea Research Institute of Chemical Technology, Korea*

Severe Acute Respiratory Syndrome Coronavirus-2 (SARS-CoV-2) continues to spread worldwide, with 25 millionconfirmed cases and 800 thousand deaths. Effective treatments to target SARS-CoV-2 are urgently needed. In thepresent study, we have identified a class of cyclic sulfonamide derivatives as novel SARS-CoV-2 inhibitors.Compound 13c of the synthesized compounds exhibited robust inhibitory activity (IC50 = 0.88 μM) againstSARS-CoV-2 without cytotoxicity (CC50 > 25 μM), with a selectivity index (SI) of 30.7. In addition, compound13c exhibited high oral bioavailability (77%) and metabolic stability with good safety profiles in hERG andcytotoxicity studies. The present study identified that cyclic sulfonamide derivatives are a promising new template for the development of anti-SARS-CoV-2 agents.



13c

- IC_{50} = 0.88 μM (Anti-SARS-CoV-2 in Vero cell)
- CC_{50} > 25 μM (Vero cell)
- Good microsomal stability
- hERG ligand binding inhibition < 1%
- Bioavailability = 77%

Poster Presentation : **MEDI.P-577**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of a novel, selective small molecule as SNF1/AMPK-related kinase (NUAK2) inhibitor for antitumor activity

Ga-young Choi[*]**, Yikyung Ko, Nam Doo Kim**[1]**, Eunhwa Ko**[2]**, Ikyon Kim, YoungSoo Kim**[*]**,**
Hwan Geun Choi[2,*]

Department of Pharmacy, Yonsei University, Korea
[1]*VORONOI BIO INC., Korea*
[2]*B2SBio, Korea*

NUAK1 (also known as AMPK-related kinase 5, ARK5) and NUAK2 (also known as sucrose non-fermenting (SNF-1)-like AMPK-related kinase, SNARK) are serine/threonine kinases belonging to AMPK (AMP-activated protein kinase) family. The NUAK kinases are reported to play important roles in tumorigenesis, metastasis, cell adhesion, cell proliferation, senescence and neuronal polarity. However, recent studies suggest that only NUAK2 in the NUAK family is related to the YAP-dependent tumors including liver, breast, bladder and so on. Because of its critical roles in biological processes, it is important to develop the inhibitors selectively targeting NUAK2. Although HTH-02-006 has been reported as the NUAK2 inhibitor (IC_{50} of NUAK2: 126 nM), it is more potent against NUAK1 (IC_{50} of NUAK1: 8 nM) than NUAK2. Therefore, we present a potent and selective inhibitor, Compound A with a novel pyrrolopyrimidine scaffold. Compound A displayed significant inhibitory effect in *in vitro* assay (IC_{50} of NUAK2: 3.46 nM). In addition, we found that Compound A displayed a 20-fold selectivity for NUAK2 over NUAK1 (IC_{50} of NUAK1: 70.22 nM). The results of the present study indicates that Compound A will serve as the development of novel targeted therapy for the NUAK2.

Poster Presentation : **MEDI.P-578**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Structure and activity relationship of pyrazolo[3,4-d]pyrimidin-1-yl piperidine derivatives as Bruton's tyrosine kinase inhibitors

Hyesu Yeom, Pilho Kim[1], Jong Yeon Hwang[2], Hyunjin Kim[3], Jae du Ha[4], Do Hyun Ryu[5,*], Sung Yun Cho[4,*]

chemistry, Sungkyunkwan University, Korea
[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*
[2]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*
[3]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*
[4]*WCI, Korea Research Institute of Chemical Technology, Korea*
[5]*Department of Chemistry, Sungkyunkwan University, Korea*

Bruton's tyrosine kinase, a non-receptor TEC family kinase, plays key role in B cell differentiation, proliferation, and survival. B cell receptor regulates the B cell's fate and cytokine release of B-lineage lymphoid leukemia cells which are deeply related with the pathogenesis of B-cell lineage of lymphoma and leukemia and autoimmune diseases. Thus, BTK protein regulation has been developed as a therapeutic target for both various cancers and autoimmune diseases. In this report, we synthesized a series of pyrazolo[3,4-d]pyrimidine derivatives that were substituted with diphenyl moieties and evaluated BTK kinase inhibitory activity and cell based proliferation assay. Some of the compounds displayed excellent activity in vitro enzymatic and cell-based assay and structure-activity relationship of the substituents will be discussed.

Poster Presentation : **MEDI.P-579**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Anti-inflammatory Effect of Phloroglucinol Derivatives Attenuates Cognitive Impairment in a LPS-Induced Mouse Model

Jushin Kim, Ki Duk Park[1,*]

Convergence Research Center for Diagnosis, Treatment and Care system of Dementia, Korea Institute of Science and Technology, Korea
[1]*Convergence Research Center for Dementia, Korea Institute of Science and Technology, Korea*

Neuroinflammation is an inflammatory immune response that occurs in the central nerve system. It is one of the important causes in neurodegenerative diseases, such as Alzheimer's and Parkison's diseases. Phloroglucinol (PG) is a natural product from brown algae and has been reported to have an anti-inflammatory effect. In this study, we synthesized derivatives of PG based on the chalcone scaffold to increase the activity of anti-inflammation. KDS4156, one of the derivatives of PG, suppressed the production of inflammatory molecule nitric oxide (NO) more effectively than PG. Furthermore, KDS4156 dose-dependently reduced expression of pro-inflammatory cytokines such as TNF-α, IL-6, IL-1β and NO producing enzyme iNOS in the LPS-stimulated BV-2 microglial cells. We also confirmed that KDS4156 did not exhibit significant cytotoxic activity compared to PG. Finally, we conducted Y-maze test, open field test and immunostaining in LPS-induced mouse model to confirm its effect in vivo. As a result, KDS4156 alleviated cognitive impairment and glial activation. These findings suggest that KDS4156, a derivative of PG, could be a potential treatment for neurodegenerative diseases.

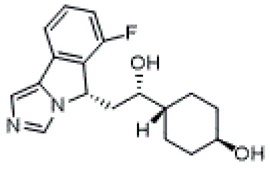
Poster Presentation : **MEDI.P-580**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and Evaluation of Imidazoisoindole Derivatives as Idoleamine 2,3-Dioxygenase 1(IDO1) Inhibitors

Jisoo Kim, Seong Hwan Kim[1], Jung-Nyoung Heo[1,*]

Graduate School of New Drug Discovery and Development, Chungnam National University, Korea
[1]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

IDO1 is an enzyme that breaks down tryptophan in the kynurenine pathway responsible for immunosuppression. Indoleamine-2,3-dioxygenase-1 (IDO1) plays an vital role in regulating the immune system through rate-limiting in kynurenine pathways. Many studies have shown that abnormal expression of IDO1 is linked to tumor cells that break down the immune system. Drugs with imidazoisoindole structure have been reported to be effective in inhibiting IDO1. Of these, Navoximod (GDC-0919; NLG-919) is a potential idoleamine-2,3)-dioxygenase pathway inhibitor and Ki/EC50 is 7nM/75nM. In this study, imidazoisoindole derivatives linked with amide, urea, and thiourea were synthesized and their IDO1 activities were evaluated.



Navoximod

Poster Presentation : **MEDI.P-581**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of Highly Potent Bruton’s Tyrosine Kinase Degraducers

Vineetkumar bapusaheb Patil, Ye Seul Lim[1], Hoyeong Park[2], Santosh Shivanand Raikar[3], Yunha Choi[4], Hyesu Yeom[5], Hyunjin Kim[6], Jae du Ha[7], Sung Yun Cho[7], Jong Yeon Hwang[8], Song Hee Lee[1], Pilho Kim[9,*]

Medicinal Chemistry, University of Science & Technology / KRICT, India
[1]*UBIX THERAPEUTICS, Korea*
[2]*Medicinal Chemistry, University of Science & Technology / KRICT, Korea*
[3]*Medicinal Chemistry, KRICT, Korea*
[4]*Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea*
[5]*chemistry, Sungkyunkwan University, Korea*
[6]*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*
[7]*WCI, Korea Research Institute of Chemical Technology, Korea*
[8]*Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea*
[9]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Bruton’s Tyrosine Kinase (BTK) is one of the most important non-receptor kinases that plays a major role in B cell receptor (BCR) signalling pathway, which is responsible for proliferation and survival of leukemic cells. Hence, targeting the BTK protein has been proved efficient for the treatment of B-cell mediated cancers, such as chronic lymphocytic leukaemia and mantle cell lymphoma. Three small molecule BTK inhibitors, ibrutinib, acalabrutinib, and zanubrutinib, have been approved by the FDA and other regulatory bodies for the treatment of B-cell related cancers. However, it was reported that resistance to ibrutinib therapy emerged mainly due to C481 mutations, hence, addressing the resistance issue has become the spotlight in this field. In this context, BTK protein degradation has shown promising results by degrading wild-type and mutants of BTK as well as inducing immunomodulatory effects. Recently, NURIX Therapeutics has developed two orally available BTK degraders, NX-2127 and NX-5948, which are in Phase 1 and preclinical studies, respectively. Encouraged by these results, we ventured into developing our own BTK degraducers. We discovered a highly potent lead compound which was more active than MT-802, a known BTK degrader. The biological data and the discovery strategy will be presented.

Poster Presentation : **MEDI.P-582**

Medicinal Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Development of pH-sensitive fluorescent probes based on reduced rhodol for imaging of lysosomes

Kunal More, Dong-Jo Chang*

Department of Pharmacy, Sunchon National University, Korea

- Withdrawal -

Poster Presentation : **MEDI.P-583**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Neuroprotective Effect of Dithiolethione-peptide Hybrids on Glutamate-induced Neurotoxicity in HT22

Yunjeong Son, Yeweon Yeon[1], Jae Wook Lee[2], Chung-Min Park*

Chemistry, Gangneung-Wonju National University, Korea
[1]*chemistry, Gangneung-Wonju National University, Korea*
[2]*Convergence Research Center for Dementia DTC, Korea Institute of Science and Technology, Korea*

Hybrids of a long-term and slow-releasing hydrogen sulfide donor ADT-OH combined with biologically active tripeptides were synthesized. The hybrids were evaluated for their neuroprotective effects on hippocampal neuron HT22 cells against glutamate-induced injury at the concentration of 3-100 μM. The cellular level of Ca^{2+} was evaluated by image analysis using the fluorescent probes Fluor-3. Reactive oxygen species (ROS) levels were examined by 2’,7’-dichlorodihydrofluorescein diacetate (DCFDH) and apoptosis inducing factor (AIF) by immunofluorescence, respectively. The occurrence of apoptotic and dead cells was determined by flow cytometry. Pre-treatment with one of the hybrids C112 significantly attenuated the glutamate-induced cytotoxicity in HT22. C112 exhibited more potent neuroprotective activity than each component ADT-OH and biologically active peptide for the hybrid. It had much less cytotoxicity to the cells at all the test concentrations than that observed with hydrogen sulfide releasing ADT-OH and peptides. Herein, we report that the hybrid C112 exerted neuroprotective effects on HT22 cells via the inhibition of the oxidative damage against glutamate-induced excitotoxicity.

Poster Presentation : **MEDI.P-584**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Study of fluoscence platform for the development of cleavable linkers using activatable fluorescent probes for leucine aminopeptidase

Dong-Jo Chang

Department of Pharmacy, Sunchon National University, Korea

Ligand targeted-drugs (LTDs) such as antibody-drug conjugates (ADCs) have been developed for the enhancement of selective localization of small molecule drugs or imaging agents into tumor tissues. In LTDs, targeting ligands as a vehicle for specific delivery to cancer cells is conjugated with a therapeutic or imaging agent via a spacer and cleavable or non-cleavable linker. Monoclonal antibodies, peptides and small molecules specific to malignant antigens have been considered as a vehicle to selectively deliver a cargo such as cytotoxic payloads to target cells as shown in ADCs. In this study, we conducted a model study for the development of cleavable linker using the activatable fluorescent probes releasing a fluorophore by the response to a oncogenic lysosomal peptidase, leucine aminopeptidase (LAP). LAP-responsive activatable fluorescent probes was designed and synthesized by the conjugation of a leucine residue to various types of xanthene fluorophores through diverse linkages with or without p-aminobenzyloxy spacer. Comparative analysis for the stability and effect of linkages and spacer on the fluorophore release was performed by the quantitative kinetic study on enzymatic and cell-based assay in HepG2 cells. The stability of the leucine linker conjugated via various linkages and spacer was evaluated ex vivo by estimating fluorescence emitted in plasma. To conclude, the activatable fluorescent probes responding to oncogenic enzymes can be used as a fluorescence platform for the development of cleavable linker in LTDs such as ADC.

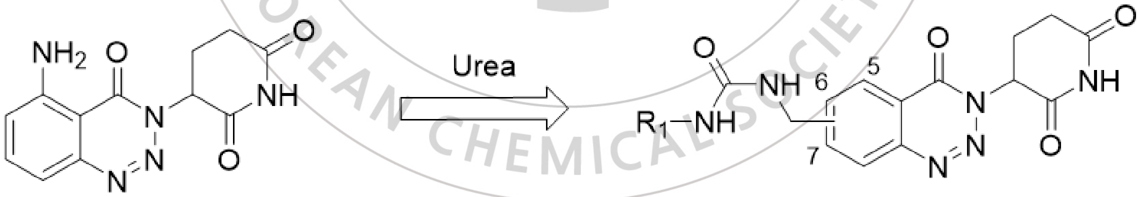
Poster Presentation : **MEDI.P-585**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of novel GSPT1 degrader based on benzotriazinone scaffold

Eunyeong Kim, Akshay Takwale, Jong Yeon Hwang[1,*]

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

The immunomodulatory drugs, lenalidomide and pomalidomide bind to cereblon E3 ligase as molecular glues and induced the degradation of neo-substrate proteins. In this study, we summarized structure-activity relationship studies of novel GSPT1 degrader, utilized with benzotriazinone scaffold. Our results propose that 6- and 7-position based urea derivatives exhibit good anti-proliferative activity than with 5-position based urea analogues in both AML (KG1) and DLBCL (TMD8) cell lines. Finally, we noticed that 6- and 7-position based urea analogues can induce the effective degradation of know neo-substrates, GSPT1, and Ikaros but not CK1a protein in KG1 cell line.



(TD-106)

Novel GSPT1 degraders

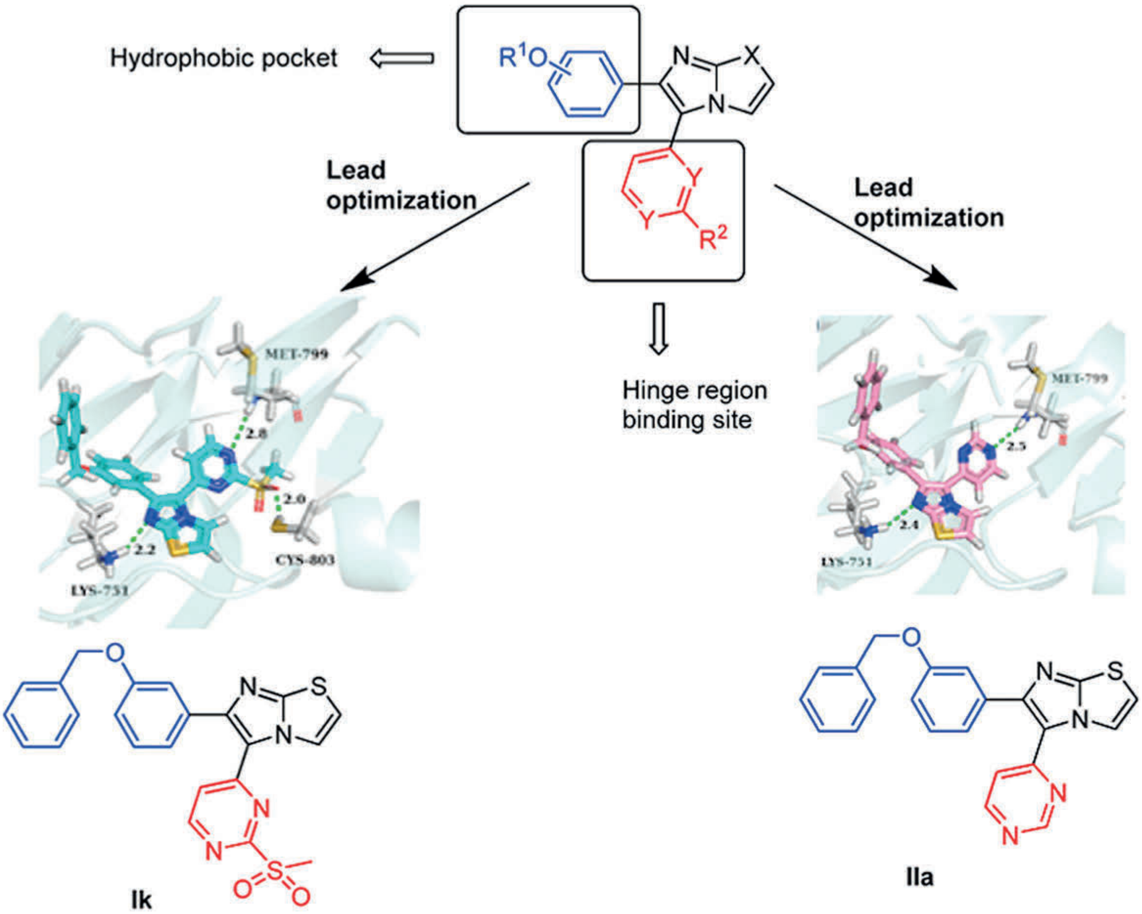
Poster Presentation : **MEDI.P-586**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of first-in-class imidazothiazole-based potent and selective ErbB4 (HER4) kinase inhibitors

Seyed omar Zareei, Chang Hyun Oh*

Biomedical science and technology, Korea Institute of Science and Technology, Korea

HER4 is the least known member of the epidermal growth factor receptor kinase family. The absence of a selective small-molecule inhibitor greatly contributes to the lack of studies and understanding of this family member. In the present study, we have discovered first in class selective small molecule inhibitors of HER4. Having imidazothiazole core, this novel series manifested itself as a new class of inhibitors of HER4 with striking differences with other non-selective HER4 inhibitors. Compounds **Ik** and **IIa** are the most potent ErbB4 kinase inhibitor (IC50 = 15.24 and 17.70 nM, respectively). Compound **Ik** showed promising antiproliferative activity., showing higher cytotoxicity towards cancer cell lines in comparison to normal cell lines. Its ability to penetrate T-47D cell membrane and inhibit ErbB4 kinase inside the cells has been confirmed. Moreover, both compound **Ik** and **IIa** have additional merits such as weak potency against hERG ion channels and CYP 3A4 and 2D6. Molecular docking and dynamic simulation studies were carried out to explain binding interactions



Selective ErbB4 inhibitor
IC_{50} = 15.24 nM
Promising antiproliferative activity

Selective ErbB4 inhibitor
IC_{50} = 17.70 nM

Poster Presentation : **MEDI.P-587**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

A Concise Synthetic Pathway for Almorexant Analogs

Santosh shivanand Raikar, Hoyeong Park[1], Pilho Kim[2,*]

Medicinal chemistry, University of Science & Technology, India
[1]*Medicinal Chemistry, University of Science & Technology / KRICT, Korea*
[2]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Korea*

Poster Presentation : **MEDI.P-588**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Current efforts for the identification of an Hsp90-selective degrader

Sehee Cha, Mingi Kim, Doyoung Kim, Hak Joong Kim[*]

Department of Chemistry, Korea University, Korea

Heat shock protein 90 (Hsp90) is an essential molecular chaperone in eukaryotes engaged in folding, stabilization, and degradation of over 400 client proteins. Many of the client proteins are oncogenic; therefore, Hsp90 is considered as one of the most important targets for anti-cancer therapy. However, previously developed inhibitors targeting Hsp90 failed to pass clinical trials due to the lack of efficacy, off-target toxicity, and more importantly induction of compensatory chaperone machineries including Hsp70 overexpression. In this regard, we decided to prepare Hsp90 degraders, or PROTAC molecules, to address whether the degradation approach can overcome the issues associated with inhibitors. Proteolysis targeting chimera (PROTAC) refers to a molecule that can selectively degrade protein of interest (POI) by inducing specific ubiquitination thereon. A PROTAC molecule is composed of ligands for POI and a E3 ligase conjugated with each other via a covalent linker. This poster presents our current progress in design, synthesis, and *in vitro* evaluation of various PROTAC compounds targeting Hsp90. In addition, how differently our PROTAC molecules behave compared to currently available Hsp90 inhibitors in terms of anti-cancer agents will be discussed.

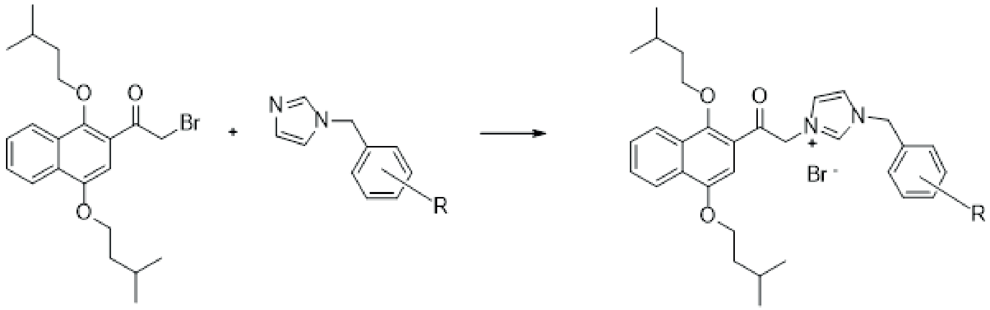
Poster Presentation : **MEDI.P-589**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Synthesis and antibacterial activity of novel hybrid 1,4-dialkoxynaphthalenacyl imidazolium salts

Chaeyun Kim, Haena Lee, Hyejin Moon, Hakwon Kim[1,*]

Kyung Hee University, Korea
[1]*Department of Applied Chemistry, Kyung Hee University, Korea*

The N-heterocycle is a general structural unit of bioactive compounds. Among them, imidazolium salt (IMS) is known as a pharmaceutical formulation exhibiting fungicidal and antibacterial activity. Previously, we reported that several synthetic IMSs containing 1,4-dialkoxynaphthalene-2-acyl moieties showed antifungal activity.In this study, we investigated synthetic naphthalenacyl-IMSs for other biological activities such as antibacterial activity. Synthetic and biological assays have been performed to confirm the antibacterial activity of several novel synthetic compounds.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Poster Presentation : **MEDI.P-590**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Study on cytoplasmic antibiotic delivery using simple bidentate siderophore mimetics

Heeyeong Lee, Do Young Kim, Hak Joong Kim[1,*]

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

The antibiotic resistance of gram-negative pathogens is a serious problem in terms of control of nosocomial infection. One of the important factors associated with the antibiotic resistance is the reduced membrane permeability. As one approach to address this issue, many research groups are testing the potential of siderophores as antibiotic delivery vehicle. In targeting gram-negative bacteria, natural siderophores are often capable of delivering the conjugated antibiotic all the way into the cytoplasm. But the difficulty in synthesis, as well as unfavorable pharmacological properties of this class of molecules, hamper their clinical development. By contrast, simple bidentate-type unnatural siderophores have been exploited as synthetically amenable and effective antibiotic delivery vectors. Nonetheless, antibiotic conjugates based on bidentate-type siderophores can only reach up to the periplasm, which significantly limits the repertoire of antibiotics to be conjugated thereto.This poster describes our strategy to overcome this limitation of artificial bidentate siderophores by enabling the cytoplasmic delivery of an antibiotic conjugate based thereon. Specifically, we hypothesized that the crossing of a siderophore-antibiotic conjugate through the inner membrane would be principally governed by its size in consideration of Lipinski rule. To test this idea, several dozens of bidentate siderophore-antibiotic conjugates whose molecular weights were controlled to be

Poster Presentation : **MEDI.P-591**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Protein membrane coated nanocomposite with medical radioisotope Zr-89 for tumor diagnosis

Jeong hoon Park*, **Jun Young Lee**

Accelerator Radioisotope Development, Korea Atomic Energy Research Institute, Korea

CD47 is a ligand that can be interacted with the SIRP-α receptor. This interaction sends to macrophage with a "Don't eat me" signal. It can inhibit the phagocytosis of macrophages. Since a large amount of CD47 is present on the surface of the red blood cell membrane (RBC$_{m}$), it can circulate blood for a long-time through interaction with SIRP- α. For enhancing tumor targeting, a biotin ligand was introduced to react with the overexpressed biotin receptor in the tumor. We report synthesizing RBC$_{m}$-coated, hollow mesoporous silica nanosphere (HMS) and biotin inserted RBC$_{m}$-HMS (BRM) with effective cancer cell accumulation. In order to evaluate the biological behavior of the nanocomposite, a diagnostic radioisotope Zr-89 was introduced. For tumor active targeting, BRBC$_{m}$ was prepared with the protein-membrane extrusion method. BRM-^{89}Zr-HMS was characterized via spectroscopic and protein quantitative/qualitative analysis. In vitro, a cancer cell internalization assay was performed to check the affinity of RBC$_{m}$-^{89}Zr-HMSN and BRM-^{89}Zr-HMS on various cancer cell lines. The results of BRM-^{89}Zr-HMS tend to increase over two days. However, RBCm$_{m}$-^{89}Zr-HMS was not showed ideal uptake, which was constantly maintained with 4.69 ± 0.13%. There is no tendency to decrease uptake, and it is maintained at a certain level. RBC$_{m}$-^{89}Zr-HMS and BRM-^{89}Zr-HMS were successfully synthesized. Base on the high level of cancer cell uptake in the in vitro experiment, the half-life in the biological system and the tumor-targeting efficiency will be evaluated through in vivo evaluation.

Poster Presentation : **MEDI.P-592**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Identification of highly potent and selective inhibitor, TIPTP, interfering the interaction of p22phox-Rubicon for treatment of rheumatoid arthritis

Sang Geon Wang, Su-Jin Gu[1], Sun-Joon Min[2,*]

Department of Applied chemistry, Hanyang University, Korea
[1]organic Medicinal Chemistry LAB, Hanyang University, Korea
[2]Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea

Rheumatoid arthritis (RA) is a chronic inflammatory autoimmune disease linked to oxidative stress, which is associated with significant morbidity. Rubicon interacts with the p22phox subunit of NOX, which is necessary for increased ROS-mediated RA pathogenesis. On the basis of a p22phox-derived peptide mimetic compound, we designed and synthesized a series of new aryl propanamide derivatives consisting of tetrahydroindazole and thiadiazole as p22phox inhibitors. After biological evaluation of these compounds, we identified 2-(tetrahydroindazolyl)phenoxy-N-(thiadiazolyl)propenamide (TIPTP, M.W. 437.44) as a lead compound, which showed high inhibitory activity of the p22phox-Rubicon interaction along with reliable in vitro stabilities and PK profile. Furthermore, we found that TIPTP displayed anti-inflammatory effects ex vivo in monocytes from healthy individuals and synovial fluid cells from RA patients. Our results suggest that TIPTP is a potential small molecule inhibitor of the p22phox-Rubicon axis and it could be applicable to the treatment of ROS-driven diseases such as RA.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **MEDI.P-593**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Development of small molecule compounds as activation for STING

Min jae Jeon, Hyejin Kim*

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

Stimulator of interferon genes (STING) is a receptor in the endoplasmic reticulum that propagates innate immune sensing of cytosolic pathogen-derived and self DNA. Activation of the STING protein by its natural ligand, cyclic guanosine monophosphate adenosine monophosphate (cGAMP), triggers signaling responses, inducing the release of type I interferons and other proinflammatory cytokines. STING-controlled interferon production is involved in antiviral defense as well as antitumor immunity. Pharmacological activation of STING is considered a promising therapeutic strategy for cancer. We designed and synthesized STING modulators and disclosed the upgraded compound 4a. Biological evaluations of compound 4a demonstrated its potency and efficacy as a direct STING agonist by *in vitro* STING binding and cell-based activity assays, thereby stimulating STING downstream signaling and efficiently promoting type I IFN immune responses. In CT26-mouse colorectal tumor model, we observed a significant reduction of tumor volume by intravenous injection of compound 4a, which revealed the remarkable therapeutic potential for cancer immunotherapy of compound 4a via STING-mediated immune activation.

Poster Presentation : **MEDI.P-594**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Optimization of baicalein's activity against *Leishmania donovani*

Ahmed Helmy Ebraheem Hassan, Suyeon Moon[1], Yeonwoo Choi[1], Yong sup Lee[2,*]

Medicinal Chemistry, Mansoura University - Faculty of Pharmacy, Egypt
[1]*Kyung Hee University, Korea*
[2]*Department of Pharmacy, Kyung Hee University, Korea*

Leishmania donovani is an intracellular parasite responsible for the majority of fatal visceral leishmaniasis. Development of potential therapeutic agents is still an unmet clinical need. Baicalein; a natural 5,6,7-trihydroxyflavone, was found to possess interesting antileishmanial activity. Baicalein stabilizes topoisomerase I–DNA cleavable complex via binding interactions different from camptothecin and inhibits camptothecin-resistant *L. donovani* promastigotes. In addition, it triggers oxidative stress and ultimate death of *L. donovani*. However, baicalein's potency as antileishmanial agent is not enough to be considered as a therapeutic candidate. Herein, optimization of baicalein to realize more potent molecules is addressed. A library of diversely-modified baicalein derivatives at rings A and C were synthesized and evaluated against *L. donovani*. Successfully, baicalein derivatives having more than 47-fold potency were achieved.

Poster Presentation : **MEDI.P-595**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery and SAR optimization of non-electrophilic antioxidant response element (ARE) activating bis-sulfones

Moonsang Yoon, Jinsook Kwak, Hwayoung Yun*

College of Pharmacy, Pusan National University, Korea

The Kelch-like ECH-associated protein 1 (KEAP1)-nuclear factor erythroid 2-related factor 2 (NRF2)-antioxidant response element (ARE) signaling pathway mediates oxidative stress resistance and hence it is considered as a promising therapeutic target for treating diseases associated with oxidative insult and senescence. A myriad of small molecules inducing ARE transcription have been reported to date: Michael acceptors, flavonoid or phenolic antioxidants, isothiocyanates, organosulfur compounds. Nearly all of these compounds are electrophilic species or have potential to transformed in cells to form electrophiles, which cause cytotoxicity. In contrast, non-electrophilic species have not treated in much detail.To this end, we recently reported CBR-470-1, a non-electrophilic bis-sulfone which promotes ARE transcription by modulating the levels of methylglyoxal, an endogenous reactive metabolite that covalently modifies NRF2 repressor KEAP1. Significant efforts have been made to develop an alternative approach towards activating ARE pathway. We designed and synthesized a novel series of bis-sulfones derived from the unique framework of CBR-470-1. Additionally, a two-step SAR optimization and detailed biological evaluation was performed to achieve highly potent and non-toxic NRF2 activation. For further modification of this scaffold, metabolite profiling was conducted to extract meticulous SAR information.

Poster Presentation : **MEDI.P-596**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

SAR studies of novel 3-benzyl-*N*-phenyl-1*H*-pyrazole-5-carboxamide derivatives as dual-acting antidiabetic agents

Jisu Kim, Jinsook Kwak, Hwayoung Yun*

College of Pharmacy, Pusan National University, Korea

Type 2 diabetes mellitus (T2DM), a pervasive disease with wide-ranging effects on social well-being, is characterized by persistent hyperglycemia caused by impaired insulin action and β-cell function, leading to serious complications. The major risk factor associated with the development of T2DM is defective glucose-stimulated insulin secretion (GSIS) in pancreatic islets. In the clinical management of T2DM, there are several antidiabetic agents currently available. However, they elicit undesirable adverse effects such as hypoglycemia, heart failure, cholangiocarcinoma and weight gain. For these reasons, identifying new molecules and pathways which can lead to the normal blood sugar level through stimulation of GSIS is urgently needed.In an effort to develop novel antidiabetic agents, an in-house chemical library was screened using INS-1 cells with a GSIS assay. From the preliminary screening, we identified a hit compound which showed a considerably enhanced insulin secretion activity. Considering the structure of hit, we designed and synthesized a series of 3-benzyl-*N*-phenyl-1*H*-pyrazole-5-carboxamides by introducing various substituents on both benzene rings. Using two-step SAR approach, we discovered a highly potent compound with enhanced GSIS from β-cells without any cytotoxicity. Western blot analysis was performed to investigate the potential mechanism of the analog. The results suggested that the analog could exhibited the increase of GSIS which mediated through the activity of pancreatic and duodenal homeobox 1 (PDX-1), an important GSIS-promoting factor. Furthermore, the analog stimulates glucose uptake via suppression of Mitsugumin 53 (MG53), an E3 ligase which is responsible for the ubiquitination of insulin receptor substrate 1 (IRS-1) in C2C12 myotube cells.

Poster Presentation : **MEDI.P-597**
Medicinal Chemistry
Exhibition Hall 1 FRI 11:00~12:30

Discovery of novel squaramide derivatives as anti-proliferative agents via activation of eIF2α phosphorylation

Jinsook Kwak, Jisu Kim, Moonsang Yoon, Hwayoung Yun*

College of Pharmacy, Pusan National University, Korea

Despite the breakthroughs in the field of cancer research over the past 100 years, pioneering of safe, non-cytotoxic, and successful cancer therapies remains an urgent task. To this end, the development of a mechanism-based anti-cancer agent that can control the complex metabolism of cancer cells has emerged as a promising solution. In eukaryotic cells, cellular proliferation, differentiation, and survival are regulated by translation initiation factors. Abnormal regulation of mRNA translation causes tumor growth and malignant transformation, involved with the development of various types of human cancers. The alpha subunit of eukaryotic translation initiation factor 2 (eIF2α) plays a critical role for the regulation of mRNA translation and protein synthesis. Phosphorylation of eIF2α restricts the formation of eIF2-GTP-Met-tRNAi ternary complex, which is crucial in the translation initiation cascade, therefore can inhibits proliferation of cancer cells.In an effort to develop potent mechanism-based anti-cancer agent, we focused on the structure of reported eIF2α kinase activator and carried out its modification by bioisosteric scaffold hopping strategy. Thus, a novel squaramide scaffold was designed, synthesized, and biologically evaluated for their effects on activation of eIF2α phosphorylation and anti-proliferative activity. Most of synthesized compounds showed potent eIF2α phosphorylation. We selected potent eIF2α activating compounds and executed CCK-8 cytotoxicity assay against K562 leukemia cells. PBMC cells was used for calculating the selectivity index (SI). From the results, we identified potent eIF2α activators which displayed high anti-proliferative activity selectively against cancer cells.

Poster Presentation : **MEDI.P-598**

Medicinal Chemistry

Exhibition Hall 1 FRI 11:00~12:30

Lateral flow assay for multiplexed nucleic acid detection using a combination of nested PCR amplicons: a new approach to combine with gold nanoparticles of LFA

Hayeon Lee

Chemistry, Incheon National University, Korea

Sepsis is a dangerous disease with a 30% rate of mortality. For a favorable recovery, it is essential to accurately diagnose and treat the infection. In order to precisely identify the pathogens, blood culture and PCR have been commonly used. In this study, we designed a method to detect infectious bacteria through multiplex PCR by combining with lateral flow assay (LFA). Recently, nucleic acid-targeting LFA has also been introduced but it is known that there are still issues on sensitivity and selectivity. For accurate and sensitive detection of disease-related nucleic acid, PCR has been considered as the gold standard, since it provides highly specific detection of target genes related to different diseases or pathogens. After PCR, amplified-nucleic acids (amplicon) results generating double-stranded nucleic acids which is not detectable with LFA. To overcome this issue, we designed a method which can be applied to LFA-based nucleic acid test by using semi-nested asymmetrical PCR. Semi-nested asymmetrical PCR uses one forward primer and two reverse primers to make different-sized PCR products. Forward primer was design that contains universal sequence at the end of 5-terminus so it can be captured with capture nanoparticles. The outer reverse primer which provides a longer PCR product and inner reverse primer which will result in a shorter PCR product. Forward primer was also designed with two different versions. The outer forward primer which contains the universal sequence and the inner forward primer without the universal sequence. To combine outer PCR products with inner PCR products for LFA, incubation process was conducted with a mixture of PCR products from both independent PCR with both sets of primers. The combinations of outer PCR products and inner PCR products have single strand ends, behaves like single strand DNA on LFA. As a proof-of-concept, target-specific primer was designed for monitoring Klebsiella pneumoniae (K.pneumoniae) and Escherichia coli (E.coli). Our results suggest that LFA-based nucleic acid test can be used for diagnostic platform as a rapid and multiplexed monitoring of pathogens by combining with PCR.

Poster Presentation : **MAT.P-316**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effect of Backbone, Length, Spacer, Substituent, Anchor, and Electrode on Thermopower of SAM

Sohyun Park, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

Understanding how the Seebeck effect of organic thermoelectric devices is associated with the chemical structure of active molecules within the devices is not only a significant challenge in chemistry but also a key goal in the research of organic and molecular thermoelectrics. This presentation describes a series of physical-organic studies that investigate structure-thermopower relationships in self-assembled monolayers (SAMs) through measurements of Seebeck coefficient (*N*, microV/K) using the eutectic gallium-indium (EGaIn)-based junction technique. Several hypotheses were derived from a transmission function-based Mott formula. These hypotheses were tested by comparing *N* values for simple alkyl and aryl molecules with different structures in terms of backbone, length, spacer, anchor, and substituent, and for different electrodes (Au vs. Ag). Experimentally obtained *N* values were further reconciled with values simulated by the Mott formula and by interfacial electronic structure and molecule-electrode coupling strength, independently measured by ultraviolet photoelectron spectroscopy (UPS) and transition voltage spectroscopy (TVS).

Poster Presentation : **MAT.P-317**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

[Withdrawal] Regeneration of Ag-M bimetallic Nanocatalysts Poisoned by Silver Halide Byproducts

Han-Jung Ryu, Jae-Seung Lee[1,*]

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

Poster Presentation : **MAT.P-318**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

[Withdrawal] One-pot Large-scale Synthesis of Polymer-capped Plasmonic Nanoparticles in Deep Eutectic Solvent

Yoon Hyuck Kim, Jae-Seung Lee[1,*]

Division of Advanced Materials Engineering, Korea University, Korea
[1] *Department of Materials Science and Engineering, Korea University, Korea*

Poster Presentation : **MAT.P-319**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Solar-induced seawater desalination using evaporators with asymmetric characteristics

Yejin Kim, Won san Choi[1,*]

Chemical and Biological Engineering, Hanbat National University, Korea
[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

Desalination has been increasingly important in many regions of the world due to population growth and shortage of freshwater. Seawater desalination is usually considered as a reliable solution in arid regions to meet the continuously growing demands for freshwater. However, various membrane or high-priced material-based vapor generators have been extensively proposed. To address the global challenges of water scarcity and the pollution of marine eco-system, we report ubiquitous material-based evaporators for water purification and desalination.

Poster Presentation : **MAT.P-320**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Crescent-shaped amphiprotic vapor generators for seawater desalination

Yujin Seo, Won san Choi[1,*]

Chemical and Biological Engineering, Hanbat National University, Korea
[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

Solar-powered vapor generation is found as one of the promising techniques for seawater desalination. The design of absorbent to promote and prevent evaporation and salt deposition, respectively, is the most important technique for desalination. To address these issues, we prepared absorbents with advanced structure that promote active circulation of vapor and hinder salt deposition, by redesign of the structure and chemical modification of the surface of absorbent/evaporator.

Poster Presentation : **MAT.P-321**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Exploration of rigid ancillary ligand effect for robust deep red emission in iridium(III) complexes

<u>Taehyun Kim</u>, Dasol Chung, Taiho Park[*]

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

Due to the small emissive bandgap, deep red and NIR wavelength targeting luminophores have critical challenges such as triplet-triplet annihilation and non-radiative decay by ground and excited state vibrational energies. Herein, in order to exhibit robust emission in deep red wavelength, we report two new phosphorescent iridium(III) complexes with introducing several substituents such as electron donating –CH3(Ir1-pic) and -H(Ir2-pic) groups on the N-coordinating quinolone moiety of a (benzo[b]thiophen-2-yl)quinoline cyclometalated ligand along with rigid picolinate ancillary ligands. The octahedral coordination and rigid ancillary ligand structures result in high triplet energy levels and robust deep red emission. Thereby, we deeply analyze density functional theory calculations and single crystal X-ray diffraction analyses to figure out the photophysical properties. Consequently, Ir1-pic and Ir2-pic exhibit enhanced internal quantum yields (0.48 and 0.37, respectively) and we fabricate organic light emitting diodes via solution process. The Ir1-pic and Ir2-pic based OLEDs show maximum external quantum efficiency values of 5.03% and 3.41%, respectively.

Poster Presentation : **MAT.P-322**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Study of Burn-in loss in Ternary Organic Photovoltaic System Composed of Semiconducting Polymers and Non-fullerene Acceptor Processed with Eco-friendly Solvent

Dasol Chung, Sunhee Yun, Taiho Park*

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

Ternary organic photovoltaic system using UV-crosslinked semiconducting polymer (P2FBTT-Br) and a non-fullerene acceptor (IEICO-4F) were processed with eco-friendly solvent and was studied in this work. P2FBTT-Br was exposed under UV irradiation for 150 seconds for crosslinking and 2-methylanisole dissolved it. Performance test for photovoltaics was executed at 75 °C or AM 1.5G Sun illumination for 90 h, UV-crosslinked devices with PC71BM exhibited 9.2% power conversion efficiency (PCE) and better stability on burn-in loss compared to the pristine devices. The locked-on morphology due to the crosslinking prohibits post-crystallization and post-aggregation leading to morphological degradation. When IEICO-4F was used as a non-fullerene acceptor, the burn-in caused by temperature and light was efficiently decreased due to the locked-on morphology and high miscibility of the non-fullerene acceptor (18.7% → 90.8% after 90 h at 75 °C and 37.9% → 77.5% after 90 h at AM 1.5G). The resulting crosslinked device displayed 9.4% PCE (9.8% in chlorobenzene), top value in crosslinked active materials using eco-friendly approach.

Poster Presentation : **MAT.P-323**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Design of Highly Active Carbon-Based H2O2 Production Electrocatalysts via Active Site Elucidation

June Sung Lim, Young Jin Sa[1], Sang Hoon Joo[2,*]

School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Kwangwoon University, Korea*
[2]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Hydrogen peroxide (H2O2) is an essential chemical that is widely used in chemical synthesis, pulp and paper bleaching, and water treatments. Nearly, 95% of current H2O2 is produced by the energy-intensive and expensive anthraquinone process. Electrosynthesis of H2O2 via the 2e− oxygen reduction reaction (ORR) has emerged as a promising alternative to the anthraquinone process that allows for environmentally benign, continuous, and on-site production of H2O2 from clean sources (air and water). While carbon nanomaterials have demonstrated promising activity and selectivity for H2O2 production, the lack of understanding of the catalytic active sites and key structural factors has remained a challenge. In this work, we have prepared a series of graphitic ordered mesoporous carbon (GOMC) model catalysts to investigate the active oxygen functional groups and structural factors. We have identified that the carboxyl (C–OOH) groups located at the graphitic edge carbon sites are the major active sites for the 2e− ORR and the carbonyl (C=O) groups are secondary active sites. The nanoporous carbon catalyst with abundant active edge sites and optimized structure exhibited the best H2O2 electrosynthesis performance among the reported carbon-based catalysts and excellent long-term stability (7 days) with near 100% H2O2 faradaic efficiency.

Poster Presentation : **MAT.P-324**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Controlling the Coordination Environments of Atomically Dispersed Catalysts via Reversible Ligand Exchange for Oxygen Reduction Reaction

Jinjong Kim, June Sung Lim[1], Sang Hoon Joo[*]

Department of Chemistry, Ulsan National Institute of Science and Technology, Korea
[1]*School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology, Korea*

Atomically dispersed catalysts (ADCs) or single-atom catalysts have attracted tremendous attention because of their 100% of metal atom efficiency and unique catalytic behaviors that are distinct from bulk or nanoparticle catalysts. In ADCs, the coordination structures around central metal atoms affect their catalytic activity and selectivity significantly. However, the control of coordination environments has been achieved empirically. In this work, we have developed a low-temperature ligand exchange method that allows for reversibly controlling the coordination structure of the metal center in the ADCs, which consequently modulate the oxidation state of the metal center and its catalytic activity and selectivity for oxygen reduction reaction (ORR) in a reversible manner. The CO-ligated atomically dispersed Rh catalyst exhibited ca. 30-fold higher ORR activity than the NHx-ligated catalyst, whereas the latter showed three times higher H2O2 selectivity than the former. Post-treatments of the catalysts with CO or NH3 allowed the reversible exchange of CO and NHx ligands, which reversibly tuned oxidation state of metal centers and their ORR activity and selectivity. The reversible ligand exchange reactions were generalized to Ir- and Pt-based catalysts.

Poster Presentation : **MAT.P-325**
Material Chemistry
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A glycopeptide enrichment strategy based on water-soluble gold nanoclusters functionalized with boronic acids

Soomin Ahn, Hongmei Xu, Dongil Lee*

Department of Chemistry, Yonsei University, Korea

Protein glycosylation is a fundamental and essential process in biological systems. Detection and analysis of glycopeptides is critical to the diagnosis of complex diseases. However, the heterogeneity of glycan structures and the low abundance of glycopeptides complicate the analysis. Thus, enrichment of glycopeptides is necessary prior to the detection, and the materials must effectively eliminate the interference of nonglycopeptides and enhance the selectivity to glycopeptides. In this work, boronic acid (BA) functionalized water-soluble atomically precise gold nanoclusters (AuNCs) were prepared as the enrichment materials. The synthesized AuNCs were characterized as $Au_{22}(SG)_{18}$ functionalized with 20 BA groups, where SG is glutathione. The as-prepared AuNCs have suitable stability, ultra-small size, and excellent biocompatibility. Functionalized boronic acids form reversible covalent bonds with glycans to have a great ability to selectively enrich intact glycopeptides. Here, we optimized the enrichment protocol using BA-functionalized AuNCs and verified by standard glycopeptides such as vancomycin and teicoplanin. The result showed that standard glycopeptides were successfully enriched through the optimized protocol. In addition, the material appears good selectivity by the comparison of enrichment efficiency of two standard glycopeptides with different numbers of binding sites. The proposed strategy has great potential to enrich glycopeptides effectively from human serum which will aid in the discovery of glycopeptides as disease biomarkers.

Poster Presentation : **MAT.P-326**
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Enhancement of optical gain of $MAPbI_3$ thin films passivated by 4-Fluorobenzylammonium iodide surface treatment

Hoonil Yang, Yoon-Kyu Song[1,*]

Department of Nanoscience and Technology, Seoul National University, Korea
[1]*Applied Bioengineering, Seoul National University, Korea*

Solution-processed organo-lead halide perovskite has gained attention in optoelectronic applications due to its low cost, tunable wavelength and narrow full width half maximum(FWHM). To improve the radiative recombination rate, spatial confinement of excitons should be improved by reducing the grain size. However, this causes defects such as pinholes and grain boundary gaps to increase.In this work, we used 4-fluorobenzylammonium iodide (FPMAI), a bulky organo-ammonium halide additive, for passivating the surface through recrystallization of the surface of $MAPbI_3$ thin films, thereby reduced the surface grain size and suppressing defects. FPMAI features well attaching to perovskite and has high surface coverage due to its short alkyl chain length and effect of fluorination, making it an appropriate additive to form a defect healing layer. Additionally, as the effect was demonstrated in ligand-assisted perovskite nanocrystal studies, we realized that FPMAI is an effective additive to form a small grain passivation layer. By recrystallizing the surface of bulky $MAPbI_3$ thin films with FPMAI additive, we observed that optical gain has improved with suppressing trap-assisted non-radiative recombination.As a result, under picosecond pulse pumping, the amplified spontaneous emission (ASE) threshold, which is one of the lasing properties, was reduced about 9 $\mu J/cm^2$, and the optical gain coefficient was increased from 257.8 cm^{-1} to 401.6 cm^{-1}. Furthermore, it indicates that the suppression of non-radiative recombination at surface defect sites is effectively inhibited through increasing PL intensity and PL decaying time. Our result shows that optical gain is improved through surface defect engineering, and it can be applied the light emitting devices such as lasers.

Poster Presentation : **MAT.P-327**
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Synthesis and Characterization of Nanocrystalline $Ni(OH)_2$ and NiO_x by Temperature-Controlled NH_3 Precipitation Method

Young Hee Jung, Yeong Il Kim[1,*]

Research & development center, Adchro, Korea
[1]*Department of Chemistry, Pukyong National University, Korea*

Nickel hydroxide and oxides are widely used in batteries, catalysts, electrochromic devices, solar energy conversion systems and sensors. Nickel hydroxide is also an important precursor to nickel oxide, as most of the nickel oxide is prepared by thermal conversion of hydroxide. Chemical base precipitation is most commonly used to prepare nickel oxide from nickel hydroxide because of the very low solubility of hydroxide. However, the crystal structure, composition and morphology of the hydroxide synthesized in this method is governed by several controlling factors such as solution pH, type of base and nickel salt, mixing rate of reactants, and reaction temperature. Among the base precipitation methods, ammonia precipitation allows fine control of the crystallinity and morphology of the hydroxides by forming nickel ammonia complexes and avoiding direct hydroxide formation. Although there have been several reported studies of the hydroxides prepared by NH_3 precipitation, to the best of our knowledge, systematic investigation of this method has not yet been conducted. In this presentation, we will demonstrate a systematic study of nanocrystalline nickel hydroxide prepared by NH_3 precipitation and non-stoichiometric nickel oxide thermally converted from the prepared hydroxide. The crystallinity and morphology of hydroxides and oxides largely depended on the type of the precursor nickel salt and the amount of base ammonia, not the reaction temperature. When the conversion temperature was below 400 ^{o}C, the crystallinity and stoichiometry trends of the converted nickel oxide followed the precursor hydroxide as well.

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Enhance Performance in Eco-Friendly Colloidal Nanocrystal-based Photovoltaics through Ligand Modification and Architecture Engineering

Sung Yong Bae, Hyosung Choi[1,*]

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

Despite recent advances in lead-free colloidal nanocrystals (NCs) silver bismuth sulfide (AgBiS2) have demonstrated promising aspects as Eco-friendly photoactive layer in photovoltaics (PVs). The conventional halide-treated NCs provide insufficient defect passivation and poor morphology, still limiting its renaissance. Herein, we revisit the surface chemistry of the AgBiS2 NCs treated with a variety of organic ligands and reveal that reactive amines and thiols significantly deform the surface by exfoliating metal ions, making the surface prone to ambient oxidation. In contrast, electron-withdrawing carboxylic acid of 3-mercaptopropionic acid (MPA) alleviate the reactivity of thiol, providing better surface passivation without detrimental effects. Nevertheless, insufficient electronic coupling over the NCs originating from spatial separation still inhibits electric conductivity, responsible for poor performance of the NCPVs. To deploy the advantages without adverse effects, a bi-layered NC photoactive layer with a combination of existing halide-passivated NC and an organic-passivated NC provides synergistic effect in the PV performance, attributed to a construction of cascade energetic landscape that extending depletion region and improved defect passivation. Consequently, by using 3-mercaptopropionic acid (MPA), a power conversion efficiency of 6.39% in AgBiS2 NC-based PV is demonstrated, responsible for the concurrent suppression of charge recombination and enhancement in charge extraction.

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Solvent Engineering of Colloidal Quantum Dot Inks for Scalable Fabrication of Photovoltaics

Jonghee Yang, Whikun Yi*, Hyosung Choi*

Department of Chemistry, Hanyang University, Korea

Development of colloidal quantum dot (CQD) inks enables single-step spin-coating of compact CQD films of appropriate thickness, enabling the promising performance of CQD photovoltaics (CQDPVs). Today's highest-performing CQD inks rely on volatile n-butylamine (BTA), but it is incompatible with scalable deposition methods since rapid solvent evaporation results in irregular film thickness with an uneven surface. Here, we present a hybrid solvent system, consisting of BTA and N,N-dimethylformamide, which has a favorable acidity for colloidal stability as well as an appropriate vapor pressure, enabling a stable CQD ink that can be used to fabricate homogeneous, large-area CQD films via spray-coating. CQDPVs fabricated with the CQD ink exhibit suppressed charge recombination as well as fast charge extraction compared with conventional CQD ink-based PVs, achieving an improved power conversion efficiency (PCE) of 12.22% in spin-coated devices and the highest ever reported PCE of 8.84% among spray-coated CQDPVs.

Poster Presentation : **MAT.P-330**
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A Development of New Polymer Donor for Semi-transparent Ternary Organic Photovoltaics with High-Performance

Jung Won Yoon, Hyosung Choi*

Department of Chemistry, Hanyang University, Korea

Organic Photovoltaics (OPVs) are a type of solar cell that are attracting attention because of their light weight, high flexibility, and low production cost. Among them, the OPVs having high transmittance can be used as semi-transparent organic photovoltaics (ST-OPVs) and has very good utility. However, current efficiencies of ST-OPVs are much lower than their opaque OPVs due to the limitations between photocurrent and average visible transmittance. For improve these limitations, we developed new polymer donor materials with strong absorption in NIR region, and high photon capture ability without increasing the thickness of the OPVs. Here, new polymer donors PL1 and PL2 were monitored effective absorption of NIR region, and had proper energy levels for blending with non-fullerene acceptor (NFA). PL1 showed highest efficiency of 7.54 %, its J_{SC}, V_{OC}, and *FF* were 20.41 mA cm^{-2}, 0.66 V, and 55.62 % in inverted structured PL1:Y6:PC$_{61}$BM (1.0:1.3:0.3, weight ratio). In case of PL2 system, PL2:Y6:PC$_{61}$BM (1.0:1.3:0.3, weight ratio) ternary blend presented a maximum PCE of 11.62 %, its J_{SC}, V_{OC}, and *FF* were 24.06 mA cm^{-2}, 0.70 V, and 69.12 %, respectively. These gaps are due to the stacking ability caused by the difference in the core length and the number of side chains of PL1 and PL2. PL2 had better stacking ability than PL1, formed appropriate domain, and facilitated charge transport. As a results PL2 is more suitable polymer donor material for ST-OPVs than PL1. We fabricated ST-OPVS using PL2 system and recorded a PCE of 8%. Recently, studies for higher transmittance are in progress.

Poster Presentation : **MAT.P-331**
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Coordination of ligands to transition metal complex with intermetallic bond via vapor diffusion in large scale

Jumin Park, Intek Song*

Department of Applied Chemistry, Andong National University, Korea

Quadruple bonds are unique intermetallic bonds that are found in certain transition metal complexes. Among various complexes having quadruple bonds, chromium(II) acetate has energy gap between HOMO and LUMO that depends on the basicity of axial ligands. However, the coordination of axial ligands requires air-sensitive process that deters the successful coordination of the ligands. Here, we present a new way to achieve the facile ligand coordination by vapor-phase ligands. The reaction was carried in a heating bath while continuously supplying inert gas into the vessel. As a result, the yield was greatly improved, and the crystals were obtained with quality.

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Material Chemistry
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Synthesis of metal-decorated NaLuGdF4:Yb^{3+}/Er^{3+} upconversion nanoparticle and its application

Bui The Huy

Department of Chemistry, Changwon National University, Korea

Fluorescent upconversion is an anti-Stokes process in which material emits a photon of higher energy after the absorption of low energy multiphoton. Fluorescent upconversion materials exhibit salient properties such as low harmfulness of low energy irradiation, non-photobleaching, deep penetration, and non-autofluorescence interference. In this presentation, we show the synthetic procedure of metal-decorated NaLuGdF4:Yb^{3+}/Er^{3+} upconversion nanoparticles (UCNPs) for detecting catecholamines. The characterizations of the prepared materials were detailed. The different metals were decorated on UCNPs to use as “triggers” for the specific detection. The experimental conditions were optimized for getting a low limit of detections for catecholamines, dopamine, and epinephrine.

Poster Presentation : **MAT.P-333**
Material Chemistry
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Electrowetting Properties of Whatman Filter Paper Decorated with Silver Nanoparticles and PVDF-HFP Film

Sharipov Mirkomil

Department of Chemistry, Changwon National University, Korea

In this work, we present a novel approach for uniform deposition of conductive silver nanoparticles and ferroelectric fluoropolymer poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) film onto HEC-modified Whatman No. 1 paper for preparation of electric valve. The novel method for deposition of conductive silver nanoparticles (AgNPs) via stabilization with polyvinylpyrrolidone (PVP) allowed to form silver nanoparticles exclusively on the surface of cellulose fibers while maintaining the porosity of the paper substrate. The optimum amount of silver ink deposited on an area equal $A=0.78\ cm_2$ was found to be 60 µL. This amount of silver reactive ink was sufficient to achieve a high conductivity of pattern while preserving the porosity of paper. Further deposition of PVDF-HFP on silver patterns in the form of honeycomb-like films made them more hydrophobic, lowering the rate of aqueous solution penetration. In the absence of voltage, the penetration rate of the aqueous solution was prolonged, with full penetration of 20 µL of aqueous solution in 35-45 minutes. The implementation of a voltage of 5 V or higher allowed to decrease the penetration time to approximately ten minutes, owing to the electrowetting properties. We integrated the developed AgNPs@PVDF-HPF patterns as the electro-responsive valve in the development of a stacked microfluidic device.

Poster Presentation : **MAT.P-334**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

A Series of Difluoroboron Dibenzoylmethane Complexes for Nitro Explosive Chemosensor

Sunhee Lee, Won-Sik Han*

Department of Chemistry, Seoul Women's University, Korea

Difluoroboron dibenzoylmethane complexes have been utilized in various applications, such as organic light emitting diodes, two-photon absorption, photochromic applications, near-IR probes, oxygen sensing materials, biosensing, and acid sensors. Interestingly, however, there are no examples of difluoroboron dibenzoylmethane complexes used as detectors for nitro explosives. In this study, three difluoroboron dibenzoylmethane compounds were prepared, which have different substituents at the peripheral phenyl groups varying from electron-withdrawing to electron-donating, **BF_2dbm-F**, **BF_2dbm-H**, and **BF_2dbm-OMe**. The photophysical and electrochemical properties of these compounds, along with density functional theory and time-dependent density functional theory calculations, were systematically investigated to study the structure-property relationships of these compounds. The excited state behaviors of these compounds were significantly different depending on the substituents, which resulted in variations in the fluorescence quantum yield and radiative/non-radiative decay rate constants. Finally, the BF_2dbm compounds were employed as selective chemosensors for the detection of nitro explosives by fluorescence quenching, and **BF_2dbm-OMe** showed the most efficient sensing ability for *ortho*-nitroaniline.

Poster Presentation : **MAT.P-335**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Improvement of Near-Infrared Phosphorescence of Iridium(III) Complex by Intermolecular Charge Transfer Mechanism

Hae Un Kim, Sangah Park, Taiho Park[*]

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

New near-infrared (NIR) phosphorescent iridium(III) complexes are synthesized to utilize the triplet–triplet annihilation and vibrational deactivation shown by low bandgap emitters, by anchoring various electron-withdrawing substituents on the (benzo[*b*]thiophen-2-yl)quinoline ligand. They are employed as dopants for the fabrication of PhOLEDs by hybrid solution-process, in which aggregation-induced phosphorescent enhancement (AIPE) effect of the phenyl-substituted molecule achieves external quantum efficiency (EQE) of 7.29%. The efficiency of NIR emission could be improved by the metal-to-ligand-to-ligand charge transfer (MLLCT) mechanism of the materials.

Poster Presentation : **MAT.P-336**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Modification of Carbon materials for Shuttle Effect by Introducing Porosity and Loading Metal Nanoparticles

Yelim Kwon, Su Jin Kim, Jung-ho Lee, Ji Man Kim[*]

Department of Chemistry, Sungkyunkwan University, Korea

Li-ion battery which is most commonly used has problems with low capacity, high price and possibility of explosion. Lithium sulfur battery is becoming a one of the promising alternatives. It has high theoretical energy density and low cost. Furthermore it is eco-friendly and safe. But polysulfide anions are dissolved in the repetitive charging and discharging so it makes the capacity decrease, which is shuttle effect.To minimize the shuttle effect, we modified ordered mesoporous carbon(OMC) materials. Carbon materials which have good conductivity are used with sulfur because the sulfur is non-conductive. Especially the OMC has thermal and chemical stability, high surface area and high pore volume. First, we synthesized the OMC materials with micropore by introducing silica nanoparticles. We expected that polysulfides with long chain could be blocked because of the small pore size. Also we loaded metal nanoparticles on the OMC. Nanoparticles of platinum could catalyze the reaction of polysulfides so dissolved polysulfides could be trapped.The materials were characterized by X-ray diffraction(XRD), N2-sorption, scanning electron microscope(SEM), and energy dispersive X-ray(EDX).

Poster Presentation : **MAT.P-337**
Material Chemistry
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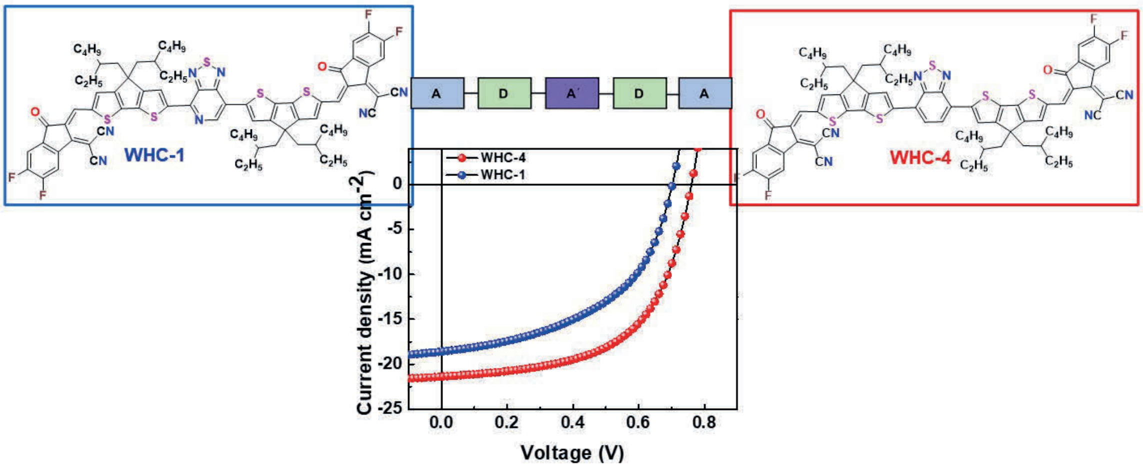
Novel Design of Non-fused Ring Acceptors based-on Pyrido- or Benzo-thiadiazole with the bandgap tuning for Organic Solar Cells

Mohammed Waseem Hussain, Hyosung Choi[*]

Chemistry, Hanyang University, Korea

Developing bulk-heterojunction (BHJ) organic solar cells (OSCs) have attracted the interest of researchers over recent past years due to their cost-effectiveness and ease of processing, advantages of transparency, lighter weight device engineering and prospect in producing large-scale OPV modules.[1] Recent breakthroughs in OSC modules exhibited high power conversion efficiencies (PCEs) exceeding over than 17% demonstrated for both single-and multijunction devices.[2] Among these prominent accomplishments, the most advantageous and emerging contributor is small molecular non-fullerene acceptors (NFAs). The popular advantages of strong and efficient light-harvesting, ease of tuning the solid-state structure and corresponding energy level are remarkable in NFAs and hence deserves as a potential candidate in OPVs.[3] However, most of the features of NFAs include a tedious multi-step synthesis with A− DD′D−A and A−DA′D−A to afford a large fused-ring backbone structure, limits their applicability to commercial fields. A simple synthetic design strategy is highly desirable to tune the solid-state microstructures and eventually their optoelectronic properties.In this work, we report a series of nonfused-rings NFAs, WHC-1 and WHC-4 based on an A−D−A′−D−A design architecture, containing an electron-deficient pyrido- or benzo-thiadiazole central unit and tailored their energy bandgap by tailoring molecular structure. Tailoring the structure by modulating the central core leads to fine-tuning of the energy levels, optical properties and molecular crystallinities. Moreover, a decent power conversion efficiency is achievable by WHC-1 and WHC-4 by blending along with PM6 polymer donor material. In the present work, we will demonstrate the potential of A−D− A′−D−A type non-fused NFAs for high-performance OSCs. Further, a structure-activity and relationship in the non-fused ring acceptors (NFRAs) could lead to tuning of their bandgap with optimized photovoltaics characteristics for high-efficiency organic solar cells.[4]


WHC-1
A
D
A'
D
A
WHC-4
WHC-4
WHC-1
Current density (mA cm^{-2})
0
-5
-10
-15
-20
-25
0.0
0.2
0.4
0.6
0.8
Voltage (V)

Poster Presentation : **MAT.P-338**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synergistic effects of Fe_2O_3 nanotube/polyaniline composites for electrochemical supercapacitor with enhanced capacitance

Farkhod Azimov, Jin Seok Lee[1], Subin Park[1], Hyun Min Jung[2,*]

Applied Chemistry, Kumoh National Institute of technology, Korea
[1]*applied chemistry, Kumoh National Institute of Technology, Korea*
[2]*Department of Applied Chemistry, Kumoh National Institute of Technology, Korea*

α-Fe_2O_3, which is an attractive material for supercapacitor electrodes, has been studied to address the issue of low capacitance through structural development and complexation to maximize the use of surface pseudocapacitance. In this study, the limited performance of α-Fe_2O_3 was greatly improved by optimizing the nanotube structure of α-Fe_2O_3 and its combination with polyaniline (PANI). α-Fe_2O_3 nanotubes (α-NT) were fabricated in a form in which the thickness and inner diameter of the tube were controlled by $Fe(CO)_5$ vapor deposition using anodized aluminum oxide as a template. PANI was combined with the prepared α-NT in two forms: PANI@α-NT-a enclosed inside and outside with PANI and PANI@α-NT-b containing PANI only on the inside. In contrast to α-NT, which showed a very low specific capacitance, these two composites showed significantly improved capacitances of 185 Fg^{-1} for PANI@α-NT-a and 62 Fg^{-1} for PANI@α-NT-b. In the electrochemical impedance spectroscopy analysis, it was observed that the resistance of charge transfer was minimized in PANI@α-NT-a, and the pseudocapacitance on the entire surface of the α-Fe_2O_3 nanotubes was utilized with high efficiency through binding and conductivity improvement by PANI. PANI@α-NT-a exhibited a capacitance retention of 36% even when the current density was increased 10 times, and showed excellent stability of 90.1% over 3000 charge-discharge cycles. This approach of incorporating conducting polymers through well-controlled nanostructures suggests a solution to overcome the limitations of α-Fe_2O_3 electrode materials and achieve performance improvement.

Poster Presentation : **MAT.P-339**
Material Chemistry
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Synthesis and Characterization of Dimeric Triphenylmethane Water-soluble Dyes for High-speed Inkjet Printing

Seong Hyun Jang, Geonho Lee, Sang Yoon Lee, Jun Choi*

Material & Component Convergence R&D Department, Korea Institute of Industrial Technology, Korea

Digital Textile Printing (DTP) is a process of printing ink with micronized dots using an inkjet printing machine to realize a designed pattern or image directly on a fabric. Digital textile printing has many advantages as follows. Firstly, it shortens the whole process time due to the elimination of screen plate manufacturing process. Secondly, it is an eco-friendly process that can reduce the environmental pollution such as waste-water. Finally, this printing method is suitable for small quantity batch production that can meet the needs of various consumers in a short time. Since DTP inks are printed with fine dots, a wider range of primary colors are required to widen the expression range of the printed pattern or image. Therefore, in this study we designed and synthesized new high-saturation deep blue color acid dyes to increase the expressive power of DTP ink. The synthesized dyes were based on modified triphenylmethane structure and calculated by the DFT method using G16 package b3lyp 6-31g (d) level, geometrical information between the moieties constituting the dye was studied. In order to improve the low water solubility of this moiety, sulfonic acid groups were introduced. At the same time, the various dimeric structures were applied to improve the light resistance and optical properties of the dyes and they were compared with the commercial blue dyes. The prepared water-based inks showed the excellent long-term storage stability by optimizing the physical and rheological properties of the inks. Moreover, they exhibited good ejection performance and well-ordered pattern arrays when applied to high-speed inkjet printing tests.

Poster Presentation : **MAT.P-340**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fast and effective synthesis of MXenes at high temperatures

Seungjun Lee, Taegon Oh[1], Chong Min Koo[1,*]

KU-KIST Graduate School of Converging Science and Technology, Korea University, Korea
[1]*Materials Architecturing Research Center, Korea Institute of Science and Technology, Korea*

Our approach towards the synthesis of various MXenes will be presented. MXenes, represented by Ti3C2Tx, have been studied extensively for a variety of applications, including energy storage, electromagnetic interference (EMI) shielding, sensors, and many others, while the vast majority of them is synthesized by hazardous HF to selectively etch A elements in MAX phases (Ti3AlC2). This reaction often takes few or more days at around room temperature. Therefore, we instead stably increase the reaction temperature up to 100 °C and thus to accelerate the etching reaction, which is not favored in coventional HF solution due to chemical hazards and the degradation of synthesized MXene. We will also show that this concept could also be applied to different types of MXenes other than Ti3C2Tx. The MXene materials synthesized by this novel method exhibit different properties such as dispersibility and surface structures.

Poster Presentation : **MAT.P-341**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Upconversion Nanoparticle Hybrid with Anisotropic Gold Nanostructures for Photonic Cancer Therapy

Subin Yu, Dong Ha Kim[*]

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

Lanthanide-doped upconversion nanoparticles (UCNP) represent a promising biomedical reagent due to their unique optical properties, converting a low energy near-infrared (NIR) light to high energy Uv-vis light. However, the practical application was limited due to their intrinsic low quantum efficiency. The integration of localized surface plasmon resonance (LSPR) has been considered as a promising way to overcome this limitation. In this contribution, titanium-coated gold nanorods (AuNR@aTiO2) were decorated with UCNP. The resulting core@shell nanostructures revealed enhanced UCNP-derived UV emission due to the plasmonic properties of AuNRs. In the presence of UCNP, the emitted UV was proposed to excite the aTiO2 and play a key role in the generation of reactive oxygen species. The introduced aTiO2 was also used as a spacer between Au NR core and UCNP to prevent the quenching of UCL. LSPR-mediated thermal effect was confirmed by temperature-rise profile. In vitro and in vivo phototherapy effect was confirmed on U87MG and the overall therapeutic effects were enhanced under the laser irradiation, confirming the combinational photothermal and photodynamic effect. Thus, our hybrid nanostructures are served as a multifunctional phototherapeutic agent in deep-range noninvasive tumor tissues

Poster Presentation : **MAT.P-342**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fast and facile fabrication of MoS2-based field-effect transistor prototype devices

Woongrae Cho, Intek Song[1,*]

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

Recently, MoS2 has been actively researched as a semiconductor material. Semiconductor devices have been made through shadow masking using metal evaporator. However, this method fails to deposit metal fast, since the evaporator requires evacuation and preparation steps. And MoS2 can be damaged soon when exposed to air, so the device should be made as quickly as possible. We quickly made a source and drain electrode using silver paint on the substrate where MoS2 and measured the FET performance. We have demonstrated that it is sufficiently possible to analyze electrical properties by making FET with silver paint, which can help save time and cost on research into devices.

Poster Presentation : **MAT.P-343**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Substituent effects on colour, aggregation, and photo-responses of trigonal molecules

Pyae myat Phyo thu, Mina Han[1,*], Longhai Piao[2,*]

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

To investigate the substituent position effect on the trigonal azobenzene molecules, we synthesized the three azobenzene derivatives with same substituents on different positions, which are three methoxy groups at (i) ortho (3oMeOAz), (ii) meta (3mMeOAz), and (iii) para (3pMeOAz) positions. Each of the compounds has different properties such as colours, solubility, shape of aggregates, and photo-responses. 3oMeOAz and 3mMeOAz are red and scarlet, respectively, while 3mMeOAz has absolutely different dark grey colour. The closer the substituents to the azobenzene moiety, the harder the solubility of the compound. The optical properties were investigated by using UV-vis absorption and fluorescence spectroscopic measurements. The self-assembled structures were fabricated in different solvents: chloroform-methanol, chloroform-hexane, N,N-dimethyl formamide-water and toluene-hexane mixed solutions and the resulting shape of the one-dimensional aggregates were analysed by optical microscopy, fluorescent optical microscopy and scanning electron microscopy observations. In addition, upon UV light irradiation, the proton signals related to the aromatic rings are shifted to upfield in 3mMeOAz while 3pMeOAz shows excellent photostability. The substituent position effect on the photo-responsive properties and morphology changes of the constructed self-assembled structures of three compounds will be reported.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **MAT.P-344**
Material Chemistry
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Preparation of red-emitting Ca(Y1-xEux)2(MoO4)4 nanophosphors for a use of transparent displays

Eung-Dab Kim, Young-Duk Huh[1,*]

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

A new synthetic method was developed for a red-emitting Ca(Y1-xEux)2(MoO4)4 (x =0.1 - 1.0) nanophosphor. The phase transfer method was used for the preparation of Ca-oleate (along with Y-oleate and Eu-oleate) and tetraoctyl ammonium (TOA)-MoO4 precursors. A hydrophobic Ca(Y1-xEux)2(MoO4)4 nanophosphor with sizes of 10 nm was obtained through the solvothermal reaction in toluene. The strong red-emission peak at 614 nm due to the 5D0 → 7F2 transition of Eu3+ was observed under the UV excitation. The stable and scattering-free suspension of Ca(Y1-xEux)2(MoO4)4 nanophosphor was obtained by simply dispersing Ca(Y1-xEux)2(MoO4)4 nanophosphor in toluene. It indicted that this nanophosphor can potentially be used as a red-emitting materials in transparent displays.

Poster Presentation : **MAT.P-345**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Discovery of Argyrodite-type novel solid state electrolyte using a metaheuristic algorithm

Sunggeun Shim, Sangwon Park[1], Woon Bae Park[1,*], Kee-sun Sohn[*], Myoungho Pyo[1,*]

Department of Nanotechnology and Advanced Materials Engineering, Sejong University, Korea
[1]*Department of Printed Electronics Engineering, Suncheon National University, Korea*

High energy density and stability have been pursued for promising lithium-ion batteries.All-solid-state batteries using solid state electrolytes(SSEs) could be a suitable alternative to liquid electrolyte lithium-ion batteries to secure high energy density, working voltage and stability.In this study, we discover novel compositions in well-known argyrodite-type SSEs that have high ionic conductivity.A metaheuristic strategy, so-called particle swarm optimization(PSO), was used for the discovery of novel argyrodite-type SSEs.An optimum set of multi-anion doping and synthesis temperature was adopted to improve ionic conductivity in the metaheuristics search process.The compound that we discovered has been analyzed by synchrotron XRD and we tested half-cell and symmetric cell performances in various conditions, and finally identified the electrochemical property.

Poster Presentation : **MAT.P-346**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Near-infrared reflective dark-tone bilayer paint system for automatic LiDAR technic

TaeHo Lim, Sangho Cho*

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

Light Detection and Ranging (LiDAR) is a representative sensor for autonomous vehicles (AVs) by detecting surrounding objects. This sensor emits near-infrared (NIR) light, usually 905 nm, and detects the reflected light. However, LiDAR has a weakness in recognizing the conventional dark-tone cars, although dark-tone is one of the most preferred colors. The typical carbon black-based dark-tone paints have low NIR reflectivity. This difficulty leads to cognitive impairment and serves as a potential car accident in the AV system. Therefore, it is necessary to develop a dark-tone paint that can be applied to LiDAR by reflecting NIR.In this work, we developed a dark-tone NIR reflective bilayer paint system: assembly of a dark-tone NIR transparent layer and a NIR reflective layer. For the dark-tone layer, we studied various combinations of organic pigments such as perylene, copper(II) phthalocyanine, and perylene bisimide derivatives. As the NIR reflective layer, we used a conventional white surfacer. After optimization, the developed bilayers exhibited dark tone with low L* values (less than 25) and high reflectivity in the NIR region, over 60%, especially at 905 nm. Therefore, we expect the developed bilayer system to be applied as a dark-tone paint detectable by LiDAR.

Poster Presentation : **MAT.P-347**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Red-emitting Single-benzene-based fluorophore-Silica Hybrid (SSH) Material

Jaehoon Kim, Dokyoung Kim[1,*]

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

Numerous fluorescent materials have been developed according to application in various fields such as basic research, industry, and medical fields. Among fluorescent materials, the development of fluorophores based on a single-benzene has recently received a lot of attention due to remarkable features i) compact size, ii) facile wavelength tuning, iii) bright blue-/green-/red-emission in solid-/solution-state, and iv) polarity-independent solvatochromic effect. Compared to other organic fluorophores, single-benzene fluorophores are relatively compact, convenient to tune wavelength, able to emit bright blue-/green-/red-light in solid-/solution-state, and showing polarity-independent solvatochromic effect. On the other side, the SBBF has its disadvantages, such as low stability under light irradiation and pH change, and limited biological application. To overcome those drawbacks, for the first time, we report a new single-benzene and silica hybrid (SSH) material that emits red fluorescence. The SSH was synthesized by one-pot reaction and it was easily converted from crude form (c-SSH) to nano-sized material (n-SSH). The physicochemical properties of the two materials were confirmed through various analyzes, and more diverse biological applications, such as bio-imaging and antibacterial effect, were presented by proving that they had better stability. Our study confirms that the hybrid of SBBF and inorganic materials can provide more diverse methods for the development of SBBF.Ref: Nanomaterials, 2021, 11, 8, 2036-2048.

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Poster Presentation : **MAT.P-348**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Metal nanocatalyst-loaded bulk catalytic filters for decomposition and conversion of organic pollutants

Won san Choi*, <u>HeeJu Kim</u>[1]

Department of Chemical & Biological Engineering, Hanbat National University, Korea
[1]*Chemical & Biological Engineering, Hanbat National University, Korea*

Metal nanocatalysts have been extensively used for synthesis of organic materials and decomposition/conversion of organic pollutants due to their excellent catalytic activity and high specific surface area. However, it has been reported that unintentional release of nanocatalysts (nano-sized particles/structures) causes serious adverse effects on humans and the environment. Thus, it is needed to develop a novel catalytic filter that does not have a risk of leakage, has a rapid catalytic reaction, high flux, easy increase/decrease in the amount of catalyst, and excellent reusability.

Poster Presentation : **MAT.P-349**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

A Janus separator for continuous and rapid oil/water separation and purification

JiHee Choi, Won san Choi[1,*]

Chemical & Biological Engineering, Hanbat National University, Korea
[1]*Department of Chemical & Biological Engineering, Hanbat National University, Korea*

Water pollution caused by domestic sewage and oily wastewater has become a serious environmental problem. Since emission regulations become stricter, oil/water separation has been increasingly important. There are various types of oil/water separation techniques, but these techniques cause time and cost limits due to the multistep separation processes. We report an amphiprotic separator with hydrophilic and hydrophobic natures for continuous and rapid oil/water separation and purification.

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October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **MAT.P-350**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Preparation of chitosan/PEO nanofibers containing carvacrol for food packaging application

Dong Hee Kim, Sang Eun Hong, Kuk Ro Yoon*

Department of Chemistry, Hannam University, Korea

Chitosan (CS)/Poly(ethylene oxide) (PEO) nanofibers membrane containing carvacrol was successfully prepared using electrospining. These nanofibers composed three different CS/PEO/Carvacrol (weight/volume) ratios and then confirmed for their physicochemical properties and food packaging effect. The carvacrol is a major component of oregano oil and has been shown to exert antimicrobial activity. We evaluated the potential application of CS/PEO nanofibers membrane containing carvacrol for fruit preservation. The morphology of the nanofibers were analysed by Field emission- Scanning electron microscope (FE-SEM). Physical and chemical properties are by Fourier transform infrared spectroscopy (FTIR), Thermogravimetric analysis (TGA), Tensile strength test, and Contact angle. The CS/PEO nanofibers contained carvacrol membrane showed promise and feasibility as an effective food preservation.**Keywords:** Nanofiber, Antimicrobial, Food-packaging, Chitosan, Carvacrol

Poster Presentation : **MAT.P-351**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Effect of Ti-doping amount on electrochromic performance of sol-gel derived WO3

Hee Sung Park, Chi-Hwan Han[1,*], Sungjun Hong[2,*], Seok In Lee[3]

Department of Energy Science and Technology, Chungnam National University, Korea
[1]*Renewable Energy Institute, Korea Institute of Energy Research, Korea*
[2]*Korea Institute of Energy Research, Korea*
[3]*Department of Chemistry, Korea University, Korea*

The electrochromic devices (ECDs) have been extensively studied because of their potential application to smart windows which can dynamically adjust indoor light and temperature of buildings. Recently, we reported that doping of WO3 with suitable Ti precursor retarded the crystallization and induced the porous networks of WO3 films, thus improving its electrochromic characteristics.1 To further optimize the amount of Ti-dopant added to WO3 precursor and post-annealing temperature, herein we varied the ratio of TCA [tetraisopropyl di(dioctylphosphate) titanate] to WO3 precursor, acetylated peroxotungstic acid (A-PTA), ranging from 0 wt% to 20 wt%. The resulting solutions were spin-coated on FTO substrate and the films were annealed at various temperature ranging from 200 to 400 °C. The combined results from SEM, XRD and in-situ optoelectrochemical measurements revealed that the best performing WO3 film was obtained with 8wt% TCA addition and 300 °C thermal treatment. The resultant WO3 films showed the high optical modulation of 70% at 550 nm and fast coloring/bleaching speed of 5.12 s and 4.87 s. In this study, we demonstrate that the optimal addition of Ti to WO3 with a proper thermal treatment can improve the electrochromic performance of WO3.Reference.1.S. Park, D. T. Thuy, S. Sarwar, H. V. Tran, S. In Lee, H. S. Park, S. H. Song, C-H. Han and S. Hong, J. Mater. Chem. C., 2020, 8, 17245-17253.

Poster Presentation : **MAT.P-352**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication of dual-band electrochromic film using oxygen deficient tungsten oxide nanoparticle synthesized by solvothermal method

Sunghyeok Park, Chi-Hwan Han*, Sungjun Hong*, Hee Sung Park[1], Seok In Lee[2]

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

The dual-band electrochromic smart window can dynamically and independently control the near infrared (NIR) and visible (Vis) light, thereby improving building energy efficiency. The studies of these dual-band electrochromic materials have been spurred by the results of complex nanocomposites such as W18O49-PB,1 PMe2T2-ITO,2 Ta or Nb-doped TiO2,3-4 and etc. However, these nanocomposites have difficulty in balancing complicated composition of each constituent. Recently, to solve these problems, research has been conducted on single component dual-band electrochromic materials, in particular, oxygen deficient tungsten oxide nanostructures.5 Most of the single component dual-band electrochromic materials have been prepared via a colloidal synthetic route under inert environment and often required a post high-temperature thermal treatment to remove the organic surfactants from metal-oxide surface, preventing their application to flexible substrates. In this study, oxygen-deficient tungsten oxide nanoparticles were synthesized by the simple solvothermal method and the highly dispersible inks were formulated which can be deposited under low temperature via various solution-based coating methods. Herein. we investigated the dual-band electrochromic characteristics of spin-coated oxygen-deficient W18O49 films which were annealed at various temperature. The XRD results showed that W18O49 films were gradually transformed to stoichiometric monoclinic WO3 structure when annealed at above 350oC, which resulted in loss of dual-band electrochromic properties. With the W18O49 films annealed at below 250oC, the cyclic voltammetry analyses in the range of -1.2V to 0.8V showed the results of good charge insertion/extraction ratio. When a moderate voltage of -0.4V was applied, the NIR light was mainly blocked with optical modulation of 23.81% and 67.27% at 550 nm and 900 nm. Further increase of the applied voltage to -1.2 V led to both blocking of Vis and NIR light with optical modulation of 71.13% and 89.60% at 550 nm and 900 nm. Moreover, these optical modulations were maintained over 1,000 consecutive cycle. We suggest in this

work a single component dual-band electrochromic material that can be useful for various applications such as electrochromic smart windows.

Reference.1.Z. Wang, Q. Zhang, S. Cong, Z. Chen, J. Zhao, M. Yang, Z. Zheng, S. Zeng, X. Yang, F. Geng and Z. Zhao, Adv. Opt. Mater., 2017, 5, 1700194.2.C. J. Barile, D. J. Slotcavage and M. D. McGehee, Chem. Mater., 2016, 28, 1439 -1445.3.M. Barawi, L. De Trizio, R. Giannuzzi, G. Veramonti, L. Manna and M. Manca, ACS Nano, 2017, 11, 3576–3584.4.S. Cao, S. Zhang, T. Zhang and J. Y. Lee, Chem. Mater., 2018, 30, 4838-4846.5.S. Zhang, S. Cao, T. Zhang, Q. Yao, A. Fisher and J. Y. Lee, Mater. Horiz., 2018, 5, 291-297.

Poster Presentation : **MAT.P-353**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Latent Fingerprint Development; Using Fluorescent Nanodiamonds to Suppress Background Fluorescence

Haksung Jung, Kyung-Jin Cho[1], Seung-Jin Ryu[2], Yasuharu Takagi[3], Paul Roche[1], Jeong Hyun Shim, Keir Neuman[4,*]

Quantum Technology Institute, Korea Research Institute of Standards and Science, Korea
[1]*National Cancer Institute, National Institutes of Health, United States*
[2]*Department of Law,Forensic Science Research Center, Korean National Police University, Korea*
[3]*National Heart, Lung, and Blood Institute, National Institutes of Health, United States*
[4]*National Heart, Lung and Blood Institute, National Institutes of Health, United States*

Owing to high sensitivity of fluorescence method, diverse fluorescent nanomaterials such as quantum dots, polymer dots, carbon dots, and up–conversion nanoparticles have been used to visualize latent fingerprints (LFPs) in forensic science. However, latent fingerprint detection using nanomaterials has faced several challenges including low sensitivity, efficiency, contrast, high background interference, and toxicity. Here we develop a new method to improve in latent fingerprint detection using poly(vinylpyrrolidone) (PVP) coated fluorescent nanodiamonds (FNDs). PVP-coated FND (FND@PVP) shows high biocompatibility at the cellular level. Due to the intrinsic amphiphilic property of PVP, FND@PVP exhibits strong interaction with LFPs. Thus, FND@PVP treated LFPs show well-defined fingerprint structures with first, second, and third level of details. Optical properties of FND@PVP induces synergetic effect to the development of LFPs with a high selectivity and a suppressed background interference. These results demonstrate that FND@PVP has great potential for high resolution and background free fluorescence imaging of LFPs using multicolor emission and dual-modal imaging.

Poster Presentation : **MAT.P-354**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Novel Ti redox-based 3D polyanion type cathode material with unprecedented cyclic stability for Ca-ion batteries

Richard Prabakar, Woon Bae Park[1,*]

Department of Printed Electronics Engineering, Sunchon National University, Korea

[1]*Department of Printed Electronics Engineering, Suncheon National University, Korea*

The practical application of calcium ion batteries (CIBs) suffer from a lack of reliable electrode materials that have long cycle-life and less severe hysteric and capacitive voltage-behavior. Here, we for the first time describe $Ti_2O(PO_4)_2(H_2O)$ as a new Ca^{2+} insertion electrode material for CIBs. Hydrothermally synthesized $Ti_2O(PO_4)_2(H_2O)$ can reversibly store ca. 0.51 Ca^{2+} (ca. 85 mAh g-1) at ca. 2.6 V vs. Ca/Ca^{2+} at room temperature. This novel material displays an unprecedented long cyclability by retaining ca. 95% of the initial capacity after 1500 charge/discharge (C/D) cycles. The structural and compositional characterizations firmly substantiate reversible Ca^{2+} insertion associated with Ti^{4+}/Ti^{3+} redox. In-situ X-ray diffraction (XRD) studies reveal that the electrochemical insertion/extraction of Ca^{2+} ions in $Ti_2O(PO_4)_2(H_2O)$ accompanies a minimal dimensional change with no transformation in the crystallographic structure, which is believed to be responsible for the exceptional stability. Bond valence site energy (BVSE) and density functional theory (DFT) calculations also demonstrate that, in contrast to reversible Li^+ insertion at ca. 1.7 V in isostructural $M_{0.5}$ $TiO(PO_4$) (M = Cu^{2+}, Mg^{2+}, Co^{2+}, Ni^{2+}, or Fe^{2+}), the significant potential upshift to 2.6 V in $Ti_2O(PO_4)_2(H_2O)$) is related to a unique Ca^{2+} location and migration path, which is ascribed to different orientations of PO_4 tetrahedra and TiO_6 octahedra.

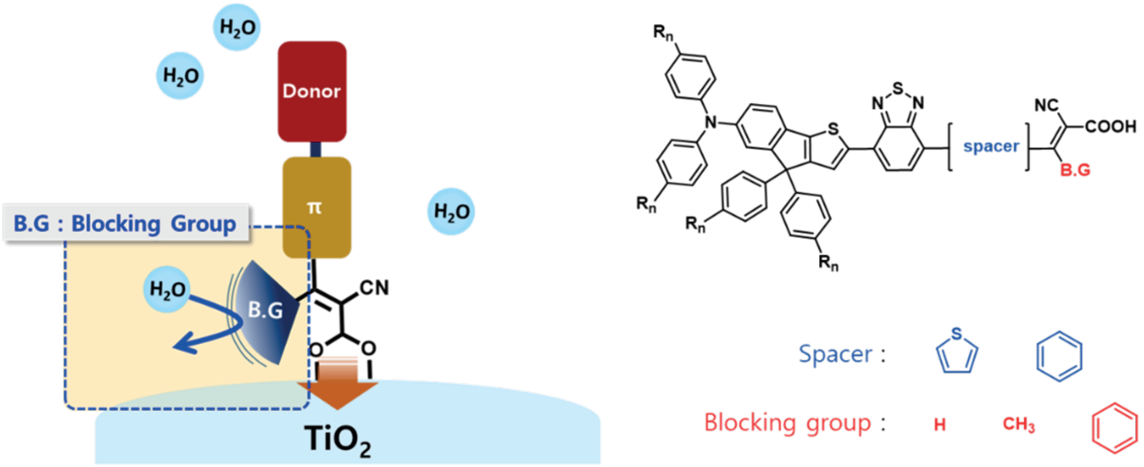
Poster Presentation : **MAT.P-355**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

PREVENTING DEGRADATION AND DESORPTION OF PHOTOSENSITZIER IN AQUEOUS CONDITION FOR VARIOUS APPLICATIONS

Tae-Hyuk Kwon*, JeongKyeong Lee

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

For emerging environmental issues, photoelectrochemical cell system to generate hydrogen molecule with solar assistance is a vital research. Cyanoacrylic acid(-CNCOOH) has been used as an acceptor and anchor to metal oxide commonly due to great electron withdrawing ability and high electron injection efficiency that can drive PEC effectively. However, by 1,4-Michael addition with H2O and direct protonation of carboxylic acid, stability of anchoring to metal oxide remarkably decreases [1]. It means that the system cannot work well. Accordingly, we have synthesized water stable acceptor with blocking groups to vulnerable reaction site so, they can physically interrupt the interactions and raise the hydrophobicity of surroundings (Figure 1). As a result, these prevent the 1,4-michael addition and also protonation of the carboxylic acid through the localized blocking effect to acceptor. To check these phenomenon, we confirmed it by UV absorption, Mass spectroscopy, Raman spectroscopy and also DFT calculations. Based on the studies, this newly designed acceptor can be applied to dye sensitized catalysis(DSC), dye sensitized photo-electrochemical cell(DSPEC) and dye sensitized solar cells(DSSCs) with long term stability.


H2O
H2O
Donor
π
H2O
B.G : Blocking Group
H2O
B.G
CN
O
O
TiO2
Rn
N
S
N S N
NC
COOH
spacer
B.G
Rn
Rn
Rn
Spacer :
S
Blocking group :
H
CH3

Poster Presentation : **MAT.P-356**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Selective adsorption of 1-octene from binary liquid n-octane/1-octene mixtures using zeolite adsorbents

Ja Yeon Kim, Chung-Yul Yoo[*]

Department of Chemistry, Mokpo National University, Korea

Linear α-olefin is a linear hydrocarbon with a double bond at the alpha position with a chemical formula CxH2x. Among Linear α-olefins, 1-octene is used as a raw material in wide range of applications, including packaging plastics, high-performing industrial oils, waxes, and surfactants. In order to obtain high purity 1-octene, the impurities with similar boiling point (i.e. n-octane and 2-octene) must be removed in the effluent stream from the catalytic reactor. In this presentation, we have conducted batch-type experiments employing 3A, 4A, 5A, and 13X zeolite beads as an adsorbent to separated 1-octene from 1-octene/n-octane binary mixture. The adsorption capacity of both 1-octene and n-octane was analyzed by gas chromatography after the adsorption experiments. The Langmuir and Freundlich adsorption isotherms were constructed to evaluated the performance of the adsorbents and interaction between the adsorbate and adsorbent. It has been observed that 3A and 4A exhibits similar adsorption selectivity for both 1-octene and n-octane, whereas 5A and 13X shows preferential adsorption of 1-octene over n-octane.

Poster Presentation : **MAT.P-357**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

N-containing Porous Aromatic Framework 41 for Improving Lithium-Sulfur Battery Performances

Qian Wang, Ji Man Kim[*]

Department of Chemistry, Sungkyunkwan University, Korea

N-containing porous aromatic framework 41 (PAF-41) with hierarchical porous structure has been readily synthesized through Scholl reaction by using triphenylamine as the monomer. The extended skeleton of PAF-41 is constructed by N-bridged biphenyl groups to generate a consecutive conjugative electronic structure. The hierarchical porous skeleton and the presence of N atoms effectively confine the electroactive species by synergistic physisorption and chemisorption to alleviate the shuttle effect that is induced by the soluble polysulfides. These features render the sulfur impregnated PAF-41 (SPAF-41) improved lithium sulfur battery performances, especially the cycling stability. SPAF-41 composite cathode with high sulfur loading of 72 wt% exhibits enhanced rate capability and excellent cycling performance. The cell delivers a high capacity of 725.8 mAh g^{-1} at 0.5 C in the first cycle and sustains a reversible capacity of 491.4 mAh g^{-1} after 500 charge-discharge cycles. A low decay rate 0.06% per cycle is achieved. The well conductive PAF-41 support bestows the cell high Coulombic efficiency of 97.36%.

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Poster Presentation : **MAT.P-358**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Intramolecular Coupling via Coupling of Au Nanoparticles and Light

Juhee Ha, Youngsoo Kim[*]

Department of Chemistry, Yeungnam University, Korea

The formation of intermolecular C-C bonds is one of the most important synthetic protocols in organic synthesis. In most molecular coupling reactions, transition metals, i.e., Pd, Ni, Cu, etc., have been used as a catalyst, and have been required high-temperature conditions and toxic organic solvent. To overcome critical issues such as harsh reaction conditions and environmental problems, various alternative synthetic strategies have been proposed. Among new ways proposed, the photocatalysis technique which uses catalysts and light could be a rational approach due to needing for mild reaction conditions and the use of less toxic chemicals. In this study, plasmonic Au nanoparticles were used as a photocatalyst and we successfully demonstrated intermolecular C-C bond formation by the plasmon-driven photocatalytic reaction. On the basis of experimental facts, we found that biphenyl, phenol, and benzene are major products. Also, we realized that the “Homo-coupling” is a more favorable pathway to form intermolecular C-C bond formation rather than the “Cross-Coupling” way in our system.

Poster Presentation : **MAT.P-359**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Plasmon Coupling on Au Nanoparticles with a Polymeric Capping Ligand

Hyeonji Kim, Youngsoo Kim*

Department of Chemistry, Yeungnam University, Korea

Plasmonic noble metal nanoparticles have distinctive properties, which indicates strong light-matter interaction. When the frequency of incident light is consistent with that of nanoparticles, the collective oscillation of conduction electrons occurs on the surface. This phenomenon is referred to as localized surface plasmon resonance (LSPR), which generates transient electron-hole pairs. These plasmonically generated charge carriers, called hot-electrons and hot-holes, can transfer to chemical species nearby and participate in redox reactions. In this study, we investigated the correlation of the electron transfer distance and photocatalytic activity on Au@PVP nanostructures. The distance between the Au core and electron acceptor was adjusted the PVP ligand thickness, resulting from the different molecular weights. Continuum electrodynamics (CED) simulation provided the rate of hot-electron generation in diverse model systems. By correlating the simulation results and the experimental facts, w elucidated the enhancing photocatalytic efficiency with shorter electron transfer distance. Consequently, we confirmed that the electron transfer reaction of plasmonic metal nanoparticles is influenced by the thickness of the ligand and the plasmon coupling phenomenon.

Poster Presentation : **MAT.P-360**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication of titanium dioxide with hollow nanostructure by electrostatic layer-by-layer self-assembly for advanced anode materials in sodium-ion batteries

Minseop Lee, Seung-Min Paek[1,*]

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

Sodium-ion batteries (SIBs) are an excellent alternative to lithium-ion batteries, and TiO_2 is an attractive electrode material due to its stability, low cost and low environmental impact. In the case of the hollow nanostructure, the easy access of the electrolyte can compensate for the slow ion diffusion of sodium ions with a larger diameter compared to lithium ions. In addition, the large buffer space can reduce the capacity loss by buffering an increase in the volume of the electrode during a long charge/discharge cycle. In this study, titanium dioxide with hollow nanostructure was successfully synthesized using electrostatic interactions between building blocks and van der Waals forces. HRTEM and PXRD analysis confirmed the crystal structure and morphology of titanium dioxide. A charge/discharge experiment and a cyclic voltammetry (CV) experiment were performed to evaluate the electrochemical properties of the electrode. It was found that the hollow nanostructure sample exhibited much better rate performance and safety compared to bulk anatase TiO_2 by having a capacity contribution by an improved pseudocapacitive process based on a large surface area accessible to sodium ions.

Poster Presentation : **MAT.P-361**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Nanoparticle grooving with sublimable liquid crystal for anti-glare film

Wantae Kim, Dong Ki Yoon[*]

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

The spontaneous assembly of nanoparticles has been used to form large-area films that perform various functions. It can be mainly applied to the design of omniphobic surfaces, semiconductor devices, and optical devices. In this study, we implemented the surface fabrication with high light transmittance and anti-glare performance using the hierarchical structure of nanoparticles. The liquid crystal mold template designed to have sublimability while maintaining the nanogroove structure can be efficiently removed by simple annealing. The fabricated nanoparticle hierarchical structure effectively scattered light incident from the side in a predictable and adjustable range. The transmittance of light in the visible wavelength range was over 90%, and the mechanical robustness by sand abrasion was also guaranteed. An additional layer may be applied to improve optical and mechanical performance, and this may be widely used in a display or a camera lens device.

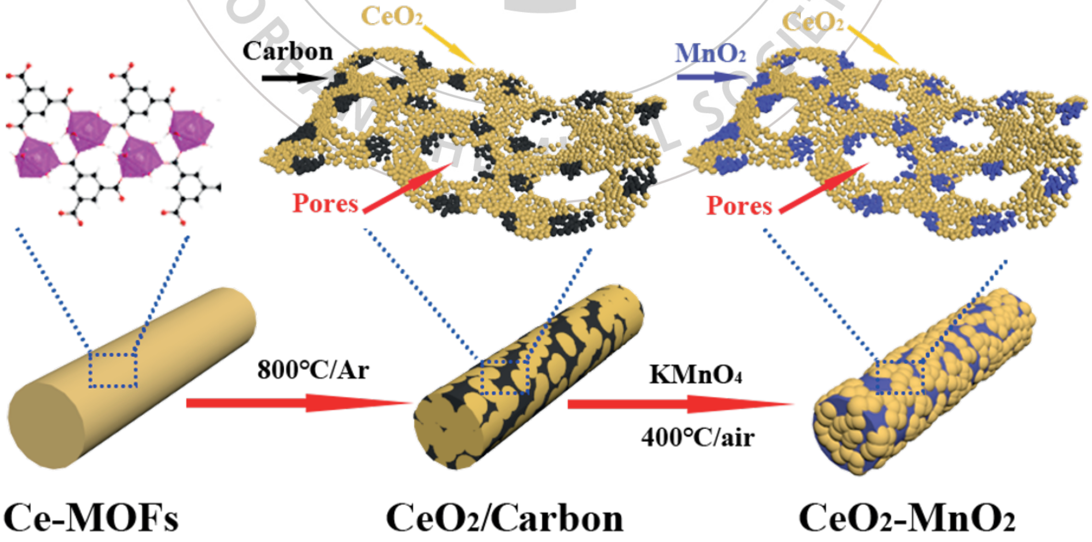
Poster Presentation : **MAT.P-362**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

MOFs derived CeO_2-MnO_2 catalysts towards CO oxidation

<u>Lianghao Song</u>, Ji Man Kim*

Department of Chemistry, Sungkyunkwan University, Korea

CeO_2-based catalysts are widely studied in the catalysis fields. Developing one novel synthetic approach to increase the intimate contact between CeO_2 and secondary species is of particular importance for enhancing catalytic activities. Herein, we design an interfacial reaction between MOF-derived Carbon and $KMnO_4$ to synthesize CeO_2-MnO_2, where the Carbon is derived from the pyrolysis of Ce-MOFs under inert atmosphere. The MOF derived Carbon is found to restrain the growth of CeO_2 crystallites at high calcination temperature, and more importantly, the intimate contact within CeO_2/C is conveyed to CeO_2/MnO_2 after interfacial reaction, which are responsible for high catalytic activity of CeO_2-MnO_2 towards CO oxidation.



Poster Presentation : **MAT.P-363**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Quercetin-Based Coating Using Amino-Quinone Networks

Sunhee Kim, Eunjung Lee, Yejin Lee, Woo Kyung Cho[*]

Department of Chemistry, Chungnam National University, Korea

Polyphenolic molecules have received great attention as universal coating precursors to design functional coatings. Various polyphenolic molecules had been screened and were found that not all molecules can serve as efficient coating precursors. Quercetin, a plant flavonol, was previously reported to be a poor coating precursor; however, we recently developed quercetin-based a substrate-independent nanocoating and demonstrated its post functionalization. Herein, as a follow-up study, we aimed to further investigate quercetin-based surface chemistry. The coating conditions were varied in terms of static/dynamic mode, temperature, the molar ratio of quercetin and an amine cross-linker, diethylenetriamine. Other amine molecules including ethylene diamine, tetraethylene pentamine, and polyethyleneimine were also utilized to examine how amino groups affect the coating efficiency. Amine molecule acted as a cross-linker to facilitate conjugate addition and imine formation with catechol in quercetin. All of the coatings were characterized by a spectroscopic ellipsometer, contact angle goniometer, X-ray photoelectron spectroscopy, atomic force microscopy, and field emission scanning electron microscopy. We found that the coating efficiency was higher under dynamic coating condition rather than static condition, and it was greatly enhanced as more amino groups were involved in the coating process. We think that our study can serve as a basis to understand polyphenol chemistry and can open a new window for engineering surface functionalization.

Poster Presentation : **MAT.P-364**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced gas sensing in drop casted Ti3C2Tx MXene sensors induced by intercalant additives

<u>Juyun Lee</u>, Chong Min Koo, Seon Joon Kim*

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

Two-dimensional (2D) metal carbide MXene has recently been studied a lot due to its excellent properties. Especially, Ti3C2Tx MXenes are attracting attention because of their high conductivity and various surface functional groups. It has been shown that gas molecules adsorb and interact much stronger on the surface of Ti3C2Tx MXene compared to other 2D materials, rendering them good candidates for gas sensing materials. Also, previous works show that the implantation of ions can further enhance the gas sensing performance. However, existing ion implantation methods and reaction enhancement methods require further research and development due to their technical complexity. In this presentation, we report a simple and cost-efficient method to tune the gas sensing properties of Ti3C2Tx, and studied the influence of acidic, neutral, and basic additives. Ti3C2Tx aqueous solutions were treated with either bases, neutral salts, or acids with similar cations and anions, which were then coated on a gas sensing electrode by drop-casting method. We show that while pristine Ti3C2Tx without any intercalants show very little reactivity to the gas sensor, Ti3C2Tx treated with bases shows high sensitivity. In particular, the gas response was the greatest in Ti3C2Tx treated with KOH for room temperature detection of NH3.

Poster Presentation : **MAT.P-365**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Oxidative modification of metal-organic framework-derived carbon: an effective strategy for adsorptive elimination of carbazole and benzonitrile

Gyudong Lee

Chemistry, Kyungpook National University, Korea

The elimination of nitrogen-containing compounds (NCCs), such as carbazole (CARB) and benzonitrile (BENZ), from fuels is essential before use. In this study, an efficient adsorbent was prepared through oxidative modification of metal-organic framework (MOF)-derived carbon to effectively remove NCCs from fuel. The prepared adsorbent, oxidized MOF-derived carbon (OMDC), showed noticeable performance in removing NCCs from model fuel. OMDC showed 4- and 26-times the adsorption capacity for the removal of CARB and BENZ, respectively, compared with that of activated carbon. Moreover, OMDC showed the highest adsorption capacity for CARB and BENZ removal compared with any adsorbent reported thus far. The adsorption process could be explained by hydrogen bonding based on the presence of many hydrogen donor and acceptor sites on the developed adsorbent. Furthermore, the adsorbent could be reused several times for NCCs adsorption after simple ethanol washing. Therefore, OMDC is a potential adsorbent for the elimination of NCCs from fuels.

Poster Presentation : **MAT.P-366**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Ionic salts@metal−organic frameworks: remarkable component to improve performance of fabric filters to remove particulate matters from air

Dong kyu Yoo

Department of Chemistry, Kyungpook National University, Korea

The elimination of particulate matters (PMs) from the air is very important for our sustainability. In this study, highly porous metal−organic frameworks (MOFs) like MIL-101 and UiO-67 were first modified, coated onto cotton, and applied in PM removal via filtration. Ionic salts (ISs) like $CaCl_2$ and LiCl, after loading onto the MOFs, remarkably increased the PM removal efficiency. For example, $CaCl_2$(20)@MIL-101/cotton shows 5.7 times the quality factor (QF, which is the most important parameter in filtration) of that of bare cotton and has the most competitive performances in PM removal (with the highest QF of 0.085 Pa^{-1} compared to any filter modified with porous materials or commercial filters. The noticeable performances of ISs@MOFs can be explained by the contribution of charge separation (that is effective for electrostatic interactions with PMs) of ISs and the high porosity of MOFs. Moreover, how MOFs with small pores of a few nanometers or less can remove large PMs with sizes in the micron range could be explained. Finally, loading ISs onto highly porous materials can be a promising strategy to improve the performances of filters to remove PMs from the air. KEYWORDS: ionic salt, mechanism, metal−organic framework, particulate matter, PMs

Poster Presentation : **MAT.P-367**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

$Na_{3-x}Sb_{1-x}W_xSe4$ as sodium-ion solid electrolytes with higher ionic conductivity

Jungyong Seo, Suyeon Han[1], Woon Bae Park[1,*]

Department of Advanced Components and Materials Engineering, Sunchon National University, Korea
[1]Department of Advanced Components and Materials Engineering, Suncheon National University, Korea

Nowadays, all-solid-state batteries (ASSBs) increasingly attract attentions as one of the most promising solutions in the endeavor for the next-generation rechargeable batteries. For the realization of commercially viable ASSBs based on Li/Li^+ chemistry, various Li^+-stuffed ISEs have been actively investigated during the last decades. Parallel to their Li counterparts, ISEs with room-temperature Na^+ conducting properties were also simultaneously studied, anticipating the applications to large-scale energy storage systems (ESSs) that necessitate the massive consumption of alkaline metals, but tolerate a somewhat low level of specific energy densities. Various oxide compounds including NASICON and β'/β''-alumina have been extensively studied, and some of those already reached the σ^{RT} of over 10^{-3} Scm^{-1}. As in Li^+ conducting ISEs, however, the high temperature sintering process to reduce grain-boundary resistance needs to be resolved for the enhancement of commercial viability. Sulfide-based Na^+ conducting ISEs, represented by Na_3MX_4 (M = P, Sb and X = S, Se), was also investigated. Hayashi et al. first reported high σ^{RT} (0.2 $mScm^{-1}$) for cubic Na_3PS_4, which had been formerly known to crystallize to a tetragonal structure with low σ^{RT} (4.17 x 10-3 $mScm^{-1}$). Their pioneering works on Na_3PS_4 have triggered intense research, including the substitution of P^{5+} and S^{2-} with more polarizable/iso-valent ions. Motivated by these recent successes, the present study describes the Na^+ conduction behaviors of W-doped Na_3SbSe_4 ($Na_{3-x}Sb_{1-x}W_xSe_4$). We select Na_3SbSe_4 as a base material because soft Se^{2-} sublattice is expected to allow the accommodation of more W^{6+} in Sb^{5+} sites and Se^{2-} anions has a tendency to be slightly oxidized, both of which contribute to the formation of Na^+ vacancies and thereby the enhancement of Na^+ conductivity. The effect of W-doping on the ionic transport is presented in this work.

Poster Presentation : **MAT.P-368**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effect of SnO_2/SiO_x impregnation on OMC as an anode for lithium ion battery

Su Jin Kim, Yun Seok Choi, Ji Man Kim*

Department of Chemistry, Sungkyunkwan University, Korea

As the demand for energy storage system increases, the development of Li secondary batteries is becoming more important. While graphite is commonly used as an anode material, it has a drawback of low theoretical capacity. The ordered mesoporous carbon (OMC) has been proven as one of the alternative anode materials with higher capacity than that of graphite, high electric conductivity, and improved rate capability. Another attractive anode materials are SnO_2 and SiO_x, which exhibit higher capacity.Here, we introduced OMC/SiO_x+SnO_2 composites by impregnation of SiO_x followed by further impregnation of SnO_2. The structure of synthesized material is characterized by XRD, N_2-sorption, SEM, and EDS. By electrochemical test, The OMC/SiO_x+SnO_2 composites showed higher electrochemical performance and rate ability than OMC/SiO_x or OMC/SnO_2 composites, or just OMC itself.

Poster Presentation : **MAT.P-369**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Highly Luminescent and Thermally Stable All-Inorganic Perovskite Nanocrystals with an Effective Defect Passivation

Geonho Lee, Sang Yoon Lee[1], Seong Hyun Jang, Jun Choi*

Material & Component Convergence R&D Department, Korea Institute of Industrial Technology, Korea
[1]*Material & Component Convergence R&D Department, Korea Institute of Industrial Technology(KITECH), Korea*

All-inorganic perovskite nanocrystals (NCs) have emerged as next-generation display materials because of their low-cost, tunable emission wavelength, high photoluminescence quantum yield (PLQY), and narrow full width at half-maximum. However, pristine perovskite NCs have low thermal stability and reduced photoluminescence due to the surface defects caused by halide vacancies. In this works, we introduced electron-rich caffeine and other imide derivatives with nitrogen and carbonyl groups to reduce surface defects in perovskite NCs. The prepared perovskite NCs with an effective defect passivation showed the improved luminescence and thermal stability. In particular, it has been reported that when mixed halide perovskite NCs are degraded, the emission wavelength is shifted due to the phase separation by halide ion migration. After heating for 1 h in 90°C, we confirmed that caffeine passivated perovskite NCs maintained the emission wavelength relatively better than pristine perovskite NCs. On the other hand, 4-Amino-N-methylphthalimide had an adverse effect. As a result of molecular calculations of caffeine and other imide derivatives, the passivation effect was consistent with the value order of the dipole moment of carbonyl oxygen. This result showed the same effect in red ($CsPbBrI_2$), green ($CsPbBr_3$), and blue ($CsPbCl_{1.4}Br_{1.6}$) perovskite NCs.

Poster Presentation : **MAT.P-370**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Terphenyl Backbone-based Geometric Isomer for Efficient Electron Transporting Material

Sanghyun Kim, Kyung-Ryang Wee[*]

Department of Chemistry, Daegu University, Korea

Three geometry isomers of the *ortho*-, *meta*-, and *para*-terphenyl backbone based benzimidazole, **o-imi**, **m-imi**, **p-imi**, for electron transporting materials (ETMs) were prepared and characterized its photophysical, electrochemical, and electron transporting properties to understand the terphenyl geometry isomer effect in the blue phosphorescence organic light emitting diodes (PHOLED). The photophysical and electrochemical properties of the three different terphenyl benzimidazole isomers were compared each other. In the absorption and cyclic voltammetry study, a gradual optical energy increase resulting from LUMO energy level changes in the order of **p-imi** < **m-imi** < **o-imi** were observed due to the each terphenyl geometry effect. Also, **o-imi** and **m-imi** isomers were showed wide band-gap with higher triplet energy ($T_1 > 2.68$ eV) because the distorted terphenyl structure (**o-imi**) and its *meta*-position non-conjugated electronic effect (**m-imi**). In contrast, **p-imi** was showed lower T_1 of 2.51 eV due to the conjugated terphenyl structure. In the DFT/TDDFT calculations, this property is explained and well agreed with experimental result.

Poster Presentation : **MAT.P-371**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Facile Intra- and Intermolecular Charge Transfer Control for Efficient Mechanofluorochromic Material

Min-ji Kim, Kyung-Ryang Wee[*]

Department of Chemistry, Daegu University, Korea

A series of donor–acceptor–donor (D–A–D) pyrene (Py) 2,7-position-based compounds (**CN**, **F**, **H**, **Me**, and **OMe**) were designed and synthesized to demonstrate facile intra- and intermolecular charge transfer control by an electron push-pull effect for efficient mechanofluorochromic (MFC) materials. An examination of the photophysical properties of **CN**–**OMe** revealed that the locally excited (LE) and intramolecular charge transfer (ICT) state of the compounds were modulated finely by the electron push-pull substituent effect. In addition, it is noteworthy that the **CN** emission originated only from the LE state despite the D–A–D molecular system. Moreover, we confirmed that the selective LE and/or ICT state modulation affects intra- and intermolecular charge transfer control in the solid-state emission. In particular, this intra- and intermolecular charge transfer control is directly dominated MFC phenomena, which means that the molecular electron push-pull substituent effect dependent MFC behavior. As a result, this study provides that as the electron-withdrawing group ability increases, the intramolecular interactions become insufficient and induce strong intermolecular D–A interactions for stabilizing molecules, leading to high MFC that are reversibly repeated several times.

Poster Presentation : **MAT.P-372**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

meta-Terphenyl Linked Donor–π–Acceptor Dyads: Intramolecular Charge Transfer Controlled by Electron Acceptor Group Tuning

Min-ji Kim, Kyung-Ryang Wee[*]

Department of Chemistry, Daegu University, Korea

A series of *meta*-terphenyl linked donor–π–acceptor (D–π–A) dyads were prepared to understand the electronic effects of a *meta*-terphenyl linker according to the electron-accepting ability change. The energy band gaps of the dyads were controlled by tuning the accepting ability, which resulted in emission colors ranging from blue-green to red. In the Lippert-Mataga plots, intramolecular charge transfer (ICT) behavior was observed, which showed gradually increased ICT characteristics as the accepting ability was increased. On the other hand, in the absorption spectra, a red shift of the ICT transition was observed differently from the electron-accepting ability tendency. Thus, the experimental results show that the ICT is determined by steric hindrance rather than the acceptor ability in the ground state due to the lack of π-conjugation of the terphenyl linker by the electron node in the *meta*-position, whereas ICT in the excited state is controlled by electron-accepting ability.

Poster Presentation : **MAT.P-373**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Ammonolytic growth of molybdenum nitride layer on Mo foil and capacitor property

Dong Hyun Lim, Young-il Kim[1,*]

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

Thin film layers of molybdenum nitrides (MoN_χ) and molybdenum dioxide (MoO_2) were grown directly on the molybdenum (Mo) foil by thermal ammonolysis. Depending on the ammonolysis temperature and time, and the post-treatment condition, MoN, Mo_2N, and MoO_2 can be obtained selectively. According to the synchrotron X-ray diffraction analysis, the above binary phases formed with nearly the same lattice parameters as the respective bulk phases, but with considerable extents of preferred orientations. Electrochemical electrodes fabricated using the MoN_χ/Mo and MoO_2/Mo foils exhibited sufficiently low interfacial resistances and high stability in aqueous acid media. The capacitor properties were examined by cyclic voltammetry and galvanoststic charge-discharge in 1 M H_2SO_4(aq).

Poster Presentation : **MAT.P-374**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Investigation of Ge-Sb substitution chemistry toward enhanced ionic conductivity for All-Solid-State Li-ion Battery.

Jihun Roh, Seung-Tae Hong[1,*]

Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science & Technology), Korea
[1]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

Sulfide inorganic materials have a potential to use solid electrolyte in Li-ion All-Solid-State-Batteries (ASSBs) due to their mechanical softness and high polarizability. In this material class, thio-LISICON Li-M-S (M=Al, P, Ge, Sn, etc.) types are composed of hexagonal closed-packed sulfide ion with multivalent metals located in the interstial sites which form Li-ion conducting framework structure. In the present study, we performed Sb^{5+} substitution on the Ge-containing sulfide structure. Structure and ionic conductivity were analyzed using X-ray diffraction, impedance spectroscopy and bond valence sum mapping (BVSM). The X-ray diffraction data shows the change of lattice parameter and solubility limit upon Sb^{5+} substitution. Considering the lattice parameter change, BVSM exhibited the decrease of Li-ion activation energy barrier, which is responsible for alleviation of bottleneck of Li^+ ion diffusion pathway. This result corresponds to increased ionic conductivity, two orders of magnitude from the pristine. By identifying the enhanced ionic conductivity, it is expected to bring the right perspective to the new composition synthesis design of solid electrolyte.

Poster Presentation : **MAT.P-375**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Nano Mo_2N embedded nitrogen-doped porous carbon, derived from phosphomolybdic acid loaded metal-azolate framework-6: an effective oxidative desulfurization catalyst

Md Mahmudul Hassan Mondol, **Sung Hwa Jhung**[1,*]

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

Nano-Mo_2N (size: ~4 nm) catalyst, well-dispersed on porous nitrogen-doped carbon, was prepared without external nitrogen sources firstly via carbonization of the phosphomolybdic acid loaded metal-azolate framework-6 (PMA@MAF-6). The prepared catalyst was applied in oxidative desulfurization (ODS) reaction in the presence of H_2O_2 as a green oxidant and showed high performance. A selected catalyst Mo_2N @CN-3 had the highest turnover frequency (30 h-1) with the lowest activation energy (27.8 KJ·mol-1) in ODS (with H_2O_2) among any molybdenum-based catalysts. The ODS over Mo_2N @CN was explained by a non-radical mechanism via active Mo-peroxo species. Moreover, the high activity of the catalyst is partly because of the contribution of nitrogen in Mo_2N. The studied catalyst could be easily recycled by solvent washing. Therefore, nano-Mo_2N @CN-3 could be suggested as a promising catalyst in ODS.

Poster Presentation : **MAT.P-376**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Nano-forensic application of latent fingerprints development using surface modified hydrophobic/fluorescent Quantum dot materials

SangJae Oh, Seung-Jin Ryu[1,*]

Investigation, Graduate School of Police Studies, Korea
[1]*Department of Law,Forensic Science Research Center, Korean National Police University, Korea*

Hydrophobic/fluorescent quantum dot nano-materials for effective development of latent fingerprints were prepared and applied to various surfaces to detect latent fingerprints. Quantum dots with fluorescence properties were coated with physically stable SiO_2, then hydrophobic quantum dots nano-materials with fluorescence and hydrophobic properties were prepared by coating the surface with polyvinylpyrrolidone. Hydrophobic quantum dot nano-materials emitted strong orange fluorescence under 365 nm ultraviolet rays, making it easier to detect latent fingerprints, especially on non-porous and semi-porous surfaces, despite the long released time of fingerprint. Based on the research results, it is expected to be used as an forensic investigative technique that can detect latent fingerprints from various surfaces than conventional dusting powder. In addition, research on DNA adsorption ability due to hydrophobic quantum dots nano-material is needed, and if DNA adsorption ability is confirmed, it is expected to be used and applicable as a strong forensic investigative technique to obtain fingerprints and DNA simultaneously.

Poster Presentation : **MAT.P-377**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Ionic conductivity of rock-salt Li_3TaO_4 depending on polymorphism and defect type

Chaeeun Kim, Young-il Kim[*]

Department of Chemistry, Yeungnam University, Korea

Ionic conductivity of complex rock-salt Li_3TaO_4 was studied using high-temperature (HT) and low-temperature (LT) polymorphs and with interstitial or vacancy defects. For each of LT and HT derivatives, four samples were prepared with different nominal compositions of $Li_{3.05}Ta_{0.99}O_4$ (L1, H1), Li_3TaO_4 (L2, H2), $Li_{2.99}Ta_{1.002}O_4$ (L3, H3), $Li_{2.98}Ta_{1.004}O_4$ (L4, H4). The synchrotron X-ray Le Bail refinement showed that the ordered HT phases have greater lattice volume than the disordered LT phases. Among both LT and HT sample groups, the lattice volume was smallest for the stoichiometric phases L2 and H2. The Li-7 solid-state magic angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy indicated that there exist two distinct chemical environments for Li in all samples. According to the ac impedance measurement and equivalent circuit analysis, both the vacancy-type and interstitial-type defects contributed to increase the ionic conductivity of Li_3TaO_4 and to similar extents.

Poster Presentation : **MAT.P-378**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Molecular Layer Deposition Behavior depending on the Crystalline Lattices of Substrate

Sung Ho Kim, Jin Seok Lee*

Department of Chemistry, Hanyang University, Korea

Previously, we conducted molecular layer deposition (MLD) of zincone films on two metal oxide substrates; SiO_2(100) and Al_2O_3 (1120) wafers. We confirmed that the surface binding energy of the substrates and the growth behavior of the films are different in the initial MLD cycles, resulting in the work functions of the zincone MLD films being different. We also propose that the difference in work functions is the result of an electron withdrawing effect due to the electronegativity of the elements. Furthermore, in previous studies, we selected Al_2O_3 wafers with various crystal graphical orientations rather than different substrates to identify the growth behavior differences.

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Poster Presentation : **MAT.P-379**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fiber Arrangement in Electrospinning Dependent on Electric Field

Ha Yun Jeong, Jin Seok Lee[1,*]

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

Electrospinning is a technology that can fabricate fibers with uniform diameters in nanoscale. These fibers can be used for tissue engineering by mimicking ECM in vivo. It is also attracting attention in many areas such as electronics by utilizing the porous properties of fiber substrates. However, it is not easy to control such as arranging the fibers using electrospinning, so it still remains a challenge. Therefore, in electrospinning, since the collector where fibers are deposited is greatly affected, many studies are being conducted to change the shape of the collector to control the fiber arrangement and change the arrangement of fibers or the amount of deposition.In this study, we designed several shapes of flat rectangular aluminum collectors through holes. By changing the size of these holes, we observed different fiber deposition and confirmed the tendency. Also, in order to analyze the cause of this trend, simulation was performed using COMSOL, and the orientation of the fiber was checked through ImageJ.

Poster Presentation : **MAT.P-380**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Uncovering The Intercalation Mechanism in Vanadium Oxide Cathode for Non-aqueous Magnesium Batteries

Dedy Setiawan, Seung-Tae Hong[1,*]

Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

Magnesium batteries have shown its promise as an alternative for lithium-ion batteries since the prototype system was suggested. The relatively low cost and high volumetric capacity of magnesium metal are the main advantages, despite the sluggish development on high energy cathode and optimization of electrolytes. So far, vanadium oxide has been demonstrated as a high capacity intercalation cathode for magnesium-ion batteries, reaching a capacity of 391 mAh g^{-1} at room temperature. However, the intercalation mechanism has not been fully understood, leaving a mystery behind such high capacity. In this presentation, we uncover the intercalation mechanism in vanadium oxide cathode using a non-aqueous electrolyte to improve the understanding on structure-to-property relationship. A combination of powder X-ray diffraction and elemental analyses was conducted reliably, suggesting pure magnesium ions intercalation into the structure. Future research direction toward high energy cathode materials for magnesium batteries will also be suggested.

Poster Presentation : **MAT.P-381**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Doped spinel cobalt oxide thin film on carbon fiber paper electrode as highly active oxygen evolution electrocatalysts

Tae Ho Kim, Soo Yeon Kim, Jong Hyeon Lee*

Department of Chemistry, The Catholic University of Korea, Korea

A crystalline thin film of metal-doped spinel cobalt oxide (M=0.01 in MxCo3-xO4) nanoparticles on a porous carbon fiber paper (CFP) electrode has been developed by the topotatic method. This hybrid is a promising combination for highly active and practical electrocatalysts used in the oxygen evolution reaction (OER). In such applications, most previous research has employed a post-annealing process to improve the particle crystallinity and an organic binder to reduce the particle size. Additionally, the conventional hydrothermal reaction of Co/Mn cations produces a mixture of metal hydroxide and metal oxide, which results in a severe drop in OER activity and stability. Here, we suggest a low-temperature (< 120 °C) and water-based thin-film fabrication process based on the deposition of cubic spinel oxide nanocrystals on a CFP electrode. This is achieved via topotactic catalysis of Co(OH)2 nanosheet that we previously developed (Dalton Trans., 2020, 49, 1652–1659). This method allows for a one-pot decoration of a spinel nanocatalyst thin-film fully covering the CFP electrode. This hybrid electrode's high performance is mainly due to the crystalline phase of the MCoO film, the exposed M cations displaying significantly more active sites on the surface, and the better contact between the spinel oxide film and the CFP electrode. Therefore, this low-temperature and aqueous process using a CFP electrode is favorable for practical OER applications.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **MAT.P-382**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Naringenin-Based, Substrate-Independent Nanocoatings

Minjin Seong, Woo Kyung Cho[*]

Department of Chemistry, Chungnam National University, Korea

Polyphenol is a kind of aromatic alcohol compound and is a natural product with several hydroxyl groups in the aromatic ring. Polyphenols are known to be associated with various health benefits, such as antibacterial, antioxidant, and anti-inflammatory properties, and are therefore in the spotlight as a functional coating material. However, not all polyphenols can act as precursors for coatings. Naringenin, which is extracted from Citrus fruit, is one of the examples of poor coating precursors. In this study, we aimed to develop naringenin-based nanocoating in a substrate-independent manner by using an amine cross-linker. Naringenin-based nanocoatings could be successfully formed on titanium oxide, gold, polytetrafluoroethylene, glass and stainless steel substrates. All of the formed films were characterized by ellipsometry, contact angle goniometry, and X-ray photoelectron spectroscopy. Furthermore, a cytotoxicity test was performed to evaluate the potential of the formed film as a biomaterial, showing that naringenin coatings are non-cytotoxic. Given the ease and versatility of coating, we think that our study can serve as a basis for understanding polyphenol chemistry and preparing functional polyphenolic coatings.

Poster Presentation : **MAT.P-383**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhancement in CO Oxidation reactivity from the Charge Transfer through the Interface between Spinel Oxide and Ceria

Jinwoung Jo, Taeghwan Hyeon[1,*]

Department of chemical and biological engineering, Seoul National University, Korea
[1]*Division of Chemical & Biological Engineering, Seoul National University, Korea*

The interfaces between an catalytic metal and an oxide support influence the catalytic reaction activity owing to the charge transfer through the interface. However, due to the complex interface structure and synthetic obstacles, the interfaces between the spinel oxide catalyst and oxide support have been less scrutinized. Herein, a synthetic strategy for controlled deposition of CeO2 layers on Co3O4, Mn3O4, and Fe3O4 nanocubes (NCs) allows us to reveal the role of the interface in catalytic CO oxidation. Strikingly, deposition of CeO2 on Co3O4 NCs enhanced CO oxidation rate up to 12- times higher than the pristine Co3O4 NCs. In situ characterization shows that the deposited CeO2 supplies oxygen through the interface to hinder the reduction of active Co3O4. The maximized charge transfer at the interface presented at the Co3O4 NCs with three facets covered by CeO2 layers which exhibit the highest CO oxidation rate even under O2-deficient conditions. The versatile change in the oxidation state was also confirmed from Co3O4 NCs with three facets covered by CeO2 layers. This study gives a nanoscale understanding of the Mars−van Krevelen mechanism occurring at the spinel oxide−CeO2 interfaces. The similar activity trend and hot electron flow are observed for oxidation of H2 using catalytic nanodiodes, thereby demonstrating that charge transfer has a critical role in the activity enhancement.

Poster Presentation : **MAT.P-384**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Selective CO_2 adsorption over functionalized Zr-based metal organic framework under atmospheric or lower pressure: contribution of functional groups to adsorption

HyeokJoon Jun

Department of Chemistry, Kyungpook National University, Korea

Selective capture of CO_2 from offgas is important to mitigate the global warming; and metal organic frameworks (MOFs) have been attractive in the capture because of huge porosity, ready functionalization and so on. In this study, a stable Zr-based MOF, MOF-808, was modified with ethylenediaminetetraacetic acid (EDTA) and further reacted with ethylenediamine (ED); and finally reduced with lithium aluminum hydride (LAH) to introduce several functional groups (FGs) onto the MOF. Moreover, the MOFs were applied in CO_2 adsorption under low pressure. The efficiency of MOF-808 in CO_2 capture was improved with EDTA loading; however, interestingly, further reaction of MOF-808-EDTA with ED causes a very much decrease in the efficiency. Importantly, the reduction of MOF-808-EDTA-ED with LAH (for MOF-808-EDTA-ED-R) leads to a remarkable increase in the performance of the MOF, for high CO_2 adsorption capacity, CO_2/N_2 selectivity and isosteric heat of adsorption. For example, MOF-808, MOF-808-EDTA, MOF-808-EDTA-ED and MOF-808-EDTA-ED-R showed CO_2/N_2 IAST selectivity (from CO_2/N_2 =15/75) of 40, 48, 19 and 197, respectively, under 298 K and 1 atm. This unusual observation could be explained with the contribution of FGs and porosity. Or, amides in cyclic rings might be formed during reaction with ED; and the MOF with amides was poor in CO_2 capture partly due to decreased porosity of the MOF; however, can be very effective in adsorption, after further reduction of amides to amines. This work shows the importance of modifications or FGs on MOFs in CO_2 adsorption, or a simple reduction can increase the adsorption selectivity as much as 10 times, which might be helpful to mitigate the global warming.

Poster Presentation : **MAT.P-385**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Platform technology for fabrication of various inorganic inverse opal photonic balls

Wonmok Lee*, Sin Geon Park

Department of Chemistry, Sejong University, Korea

Photonic crystals are substances with repeating lattice structures of similar magnitude to the wavelengths of light, which is reflected at a particular angle through Bragg diffraction. One of nature-occurring photonic crystal is an opal structure, and this study demonstrates the controlled evaporation of emulsified polystyrene nanoparticles and silica particles to obtain photonic balls in the form of 100 micron-sized beads with opal structures in large quantities respectively by water-in-oil manufacturing. Using the photonic balls as template, various inorganic inverse opal photonic balls are fabricated such as tiania, silica, and carbon.

Poster Presentation : **MAT.P-386**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Preparation of Magnetic Silica Nanotubes with Protease inside for Reusable and Sustainable Enzymatic Hydrolysis

Jieun Kim

chemistry, Gachon University Global Campus, Korea

Silica nanotubes (SNTs) interact well with a variety of bio-materials and are advantageous in creating multifunctional surfaces because the hydroxyl groups exposed to the SNTs surface are easy to react with other functional groups. This enables organic immobilization of hydrophilic or hydrophobic surface modifications and biomaterials. In addition, a large amount of tube can be manufactured by a simple fabrication method based on anodic aluminum oxide (AAO). These SNTs were applied to the immobilization of enzymes. Among enzyme types, protease, also has a limitation in immobilization technology, and since protease is a protein made up of amino acid sequences, self-digestion occurs when used for a long time. To overcome this problem, the enzyme was immobilized inside the SNTs. By immobilizing the protease with an organic bond inside the SNTs, the probability of self-decomposition is reduced and the enzyme properties can be maintained for a long time because the protease remains fixed at a certain distance. Iron oxide nanoparticles can be introduced inside this tube to enhance ease of reuse. The constructed structure was identified by SEM, TEM, and the enzyme activity of the constructed structure was confirmed by SDS-PAGE and UV-vis spectroscopy.

Poster Presentation : **MAT.P-387**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Room Temperature Synthesis of Anion-Stabilized Cubic Bismuth Oxide

Hee Sun Park, Hee Jung Yang, Jaeyeon Kim, Nam hwi Hur*

Department of Chemistry, Sogang University, Korea

Bismuth oxide (Bi2O3) has several crystallographic polymorphs. The most common structure is an alpha phase, which adopts a monoclinic symmetry. The delta phase (d-Bi2O3) has a fluorite-type cubic structure with oxygen defects and has important potentials for ceramic electronic devices due to its highest conductivity of known solid-state oxide conductors. However, a drawback is that d-Bi2O3 exists above 729 °C and is not stable at low temperature. Moreover, the structure can be retained by doping with high-valence cations such as Re7+, Mo6+, Ta5+, Nb5+, V5+, and lanthanide ions. Here we report the room-temperature synthesis of fluorine-stabilized d-Bi2O3 using various chemical means. The delta phase was fully characterized by X-ray diffraction, transmission electron microscopy, scanning electron microscopy, and X-ray photoelectron spectroscopy. A possible mechanism will also be presented to explain the formation of the anion-stabilized d-Bi2O3.

Poster Presentation : **MAT.P-388**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Unprecedented Calcium Vanadium Bronze as a Cathode Material for Calcium-Ion Batteries

Hyeri Bu, Seung-Tae Hong[1,*]

ENERGY SCIENCE AND ENGINEERING, DGIST, Korea
[1]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

Calcium-ion batteries (CIBs) are considered an attractive candidate for post-Li-ion batteries. However, there are difficulties to find intercalation-type cathode materials working with anhydrous electrolytes. Herein, we report a novel calcium vanadium bronze (CVO) as a cathode material of CIBs. CVO was synthesized via a simple electrochemical ion-exchange method. Its unique structure was determined from a powder X-ray diffraction data and electron diffraction data for the first time. It has a layered structure composed of V-O layers stacking along the c-axis and Ca ion occupying the interlayer space. Reversible electrochemical intercalation of Ca^{2+} ions into CVO has been demonstrated using galvanostatic discharge/charge cycling. The discharge capacity is reached ~120 mAh g^{-1} and showed stable cycle performance in room temperature after activation process in high temperature. On activation process, the overall rearrangement of structure occurred, while almost all Ca^{2+} ions lying in interlayer were extracted. After moved to room temperature, Ca^{2+} ions are inserted reversibly, reverting to the pristine structure. The rearrangement of structure seemed to play an important role in better cycle performance and rate capability. It shows that the activation process of the crystal structure might change the probability of cathode material totally.

Poster Presentation : **MAT.P-389**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis and Characterization of Phosphorus-Doped Mesoporous Carbon and its Application on Lithium ion Battery

Jae Ik Lee, Ji Man Kim[1,*]

Functional Material Chemistry, Sungkyunkwan University, Korea
[1]*Department of Chemistry, Sungkyunkwan University, Korea*

Heteroatom doped mesoporous carbon has recently received lots of attention due to its various advantages. Especially when it was used as anode material in lithium-ion batteries, power density • energy density • stability of an electrode increased compared to ordinary carbon anode materials. In this research phosphorus was selected as a target atom because of its positive effect on the electrode which was treated in recent researches.Phosphorus doped mesoporous carbon was synthesized using nano-replication method. SBA-15 was used as silica template and various carbon • phosphorus precursors were used. These materials were then characterized by X-ray diffraction, Nitrogen sorption isotherm analysis, FT-IR and electron microscopy.

Poster Presentation : **MAT.P-390**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Direct Investigation into Catalytic Performances of Different Active Sties on Rhombic Dodecahedral Pd Nanocrystal Catalysts

Bon Seung Goo, Jong Wook Hong[1,*], Sang Woo Han[*]

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

The existence of various surface active sites within a nanocrystal (NC) catalyst complicates understanding their respective catalytic properties and designing an optimal catalyst structure for a desired catalytic reaction. Here, we developed a novel approach that allows unequivocal investigation on the intrinsic catalytic reactivity of the edge and terrace atoms of NCs. Through the comparison of the catalytic behaviors of edge-covered Pd NCs, which were prepared by the selective deposition of catalytically inactive Au atoms onto the edge sites of rhombic dodecahedral (RD) Pd NCs, with those of the pristine RD Pd NCs toward alkyne hydrogenation and Suzuki-Miyaura coupling reactions, we could decouple the activity of the edge and {110}-plane atoms of the Pd NCs without uncertainties. We expect that this study will provide an opportunity to scrutinize the surface properties of various NC catalysts to a more precise level and devise ideal catalysts for intended catalytic reactions.

Poster Presentation : **MAT.P-391**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Ag-CdS Yolk-Shell Heteronanostructures with Spectral Overlap for Photocatalytic Hydrogen Evolution Reaction

Youngjoo Whang, Sang Woo Han[1,*]

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

The combination of a semiconductor and a plasmonic metal holds great promise for developing advanced photocatalysts. However, the realization of a heteronanostructure that accommodates both materials in an effective way has been a great challenge. Herein, we report a synthesis of a photocatalyst with a yolk-shell heteronanostructure, which contains a plasmonic Ag yolk inside a CdS shell. The sulfidation of Ag nanospheres followed by a controlled cation exchange reaction successfully generated the Ag-CdS yolk-shell nanostructures. The as-prepared heteronanostructures exhibited a prominent enhancement of photocatalytic activity toward hydrogen evolution reaction under visible-light irradiation compared to CdS hollow nanoparticles without the Ag yolk. This improvement can be attributed to the plasmon energy transfer from the Ag yolk to the CdS shell and the yolk-shell structure that enables the multiple reflections of the incident light.

Poster Presentation : **MAT.P-392**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Electrochemical and Structural studies of sodium solid electrolytes in the new substitution series.

Seung-Tae Hong*, **Dongyeon Yun**[1]

Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea
[1]*Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

The design of high-performance Na-ion solid electrolytes (SEs) is one of the key challenges to enable room temperature all-solid-state sodium ion batteries. The sulfide sodium solid electrolytes are attractive for large-scale energy storage applications due to their abundance and low cost. in addition, sulfide solid electrolytes have softer properties, making it possible to alleviate the gain boundary problem with only high pressure and because of its large ionic radius, it can effectively broaden the sodium ion transport path. In this work, we identify sodium ion conductors in the new substitution series, using the earth-abundant elements. This substitution series reveal a new X-ray diffraction pattern, indicating the structure change in solid electrolytes. The evolution of a new phase, distinctly different from based ternary materials, shows a drastically increased ionic conductivity. The unusual change is in accord with the change in the XRD patterns, which strongly indicates that the new phase is responsible for the high ionic conductivity.

Poster Presentation : **MAT.P-393**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

A potassium vanadium phosphate as a cathode material for Ca batteries

Hyungjin Lee, Hyeri Bu[1], Seung-Tae Hong[2,*]

Department of Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*ENERGY SCIENCE AND ENGINEERING, DGIST, Korea*
[2]*Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea*

Calcium-ion battery is the promising candidate for post lithium-ion batteries. For development of ca-ion batteries, finding suitable electrode material is the key. Vanadium phosphate, such as NASICON, is widely studied thanks to its robust structure, enabling fine electrochemical performance. Herein, we studied potassium vanadium phosphate, KVPO, for the first time as Ca-ion cathode material. KVPO is synthesized by facile hydrothermal method. The VO6 octahedrons are connected by PO4 tetrahedrons with corner sharing, and that slabs are staked along y direction. Guest ions move between layered slab in the x-z directions. Reversible calcium ion intercalating into KVPO is demonstrated by using galvanostatic electrochemical test with homemade cell. The discharge capacity is around 100 mAh g-1 and it showed reversible cyclability for many cycles. During charge and discharge cycle, the structure change is determined by powder X-ray diffraction (XRD). It showed reversible peak shift during cycle. During charge process, little amount of ions are stuck in host material, which seems to make the structure more stable and better cyclability. During discharge process, only target ion is inserted to structure, reversibly. Excluding the possibility of proton intercalation and existence of crystal water are determined by thermogravimetric analysis (TGA). The results show that KVPO is a potential host material for Calcium-ion batteries.

Poster Presentation : **MAT.P-394**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Optimized Ultrasonication Method for Synthesizing Highly Luminescent Cesium Lead Halide Perovskite Nanocrystals

Sang Yoon Lee, Geonho Lee, Seong Hyun Jang, Jun Choi[*]

Material & Component Convergence R&D Department, Korea Institute of Industrial Technology, Korea

Optical materials based on halide perovskite nanocrystals have received widespread attention in recent years. One of the main advantages of these materials is the fact that the optical band gap can be easily tuned by exchanging individual components. These materials quickly led to the synthesis of nanocrystals, first in the form of organic/inorganic hybrid perovskites, and later also as purely inorganic cesium-based perovskites. But the practical applications of perovskite nanocrystals have been limited by their poor stability. In addition, conventional methods such as hot injection method and ligand-assisted re precipitation method are difficult to manufacture on a large scale due to complex conditions and long synthesis time. Thus, we suggest the simple, scalable, single-step, and polar-solvent-free synthesis of high-quality colloidal $CsPbX_3$(X= Cl, Br and I) perovskite nanocrystals with tunable halide ion composition by direct ultrasonication of the corresponding precursor solutions. The synthesized nanocrystals exhibit high photoluminescence quantum yields, narrow emission line widths, and considerable air stability. This study provides a valid route toward highly stable, extremely emissive, and panchromatic perovskite nanocrystals with potential use in a variety of future optoelectronic applications.

Poster Presentation : **MAT.P-395**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

High thermoelectric properties of hole doped-polycrystalline $Sn_{1-x}Ge_xSe$

Taeshik Kim, Chung In[1,*]

IBS center for correlated electron systems(CCES) and school of chemical and biological engineering, Seoul National University, Korea
[1]*School of Chemical & Biological Engineering, Seoul National University, Korea*

Thermoelectric (TE) materials are promising technologies because they can convert waste heat directly into electrical energy. SnSe single crystals have shown exceptionally high thermoelectric figure of merit (ZT) of ~2.6 at 923K along the b-axis due to a highly anharmonic bonding. However, it is inefficient because it takes time and cost to obtain high quality. Although polycrystalline SnSe has lower performance compared to single crystal samples, it has advantages of machinability and scalability, so it is advantageous for device applications. Therefore, achieving TE properties of polycrystalline SnSe samples similar to or higher than single crystal samples are one of the most important reserch. However, it is quite difficult to make a high ZT polycrystalline SnSe material because of both low dopability and solubility limit with other elements.In this presentation, we investigated the effect of Ge substitution for Sn on the TE properties of p-type Sn1-xGexSe. We demonstrate that a delicate control of Ge alloying in SnSe gives a higher Seebeck coefficient by controlled phase change temperature and also a lower thermal conductivity. As a result, the best performing system achieves a high ZT of 1.4 at 800K.

Poster Presentation : **MAT.P-396**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Realizing unusual low thermal conductivity of chalcopyrite In-doped $CuFeS_2$ system by local structure manipulation

Hyungseok Lee, Bangzhi Ge[1], Chung In*

Center for Correlated Electron Systems (IBS) and School of Chemical and Biological Engineering, Seoul National University, Korea

[1]*State Key Laboratory for Mechanical Behavior of Materials, Xi′an Jiaotong University, China*

Chalcopyrite-type compounds have been studied for nonlinear optics and photovoltaics. $CuFeS_2$, the representative of the chalcopyrite-type compounds, consist of cheap and eco-friendly elements. However, due to high lattice thermal conductivity(κ_L), thermoelectric application of the chalcopyrite has been limited. If suitable strategies for reducing κL are applicable, $CuFeS_2$-based materials can be a promising thermoelectric material.Herein, we report the integrated strategies for decreasing κ_L of $CuFeS_2$ system by introducing In. Incorporated In in Cu site has $5s^2$ lone pair electrons and induces atomic disorders among atoms with similar ionic radii. These strategies for local structure manipulation contribute to phonon softening, which dramatically reduces κ_L. Consequently, 8 % In-doped $CuFeS_2$ shows decreased κ_L of ~2.60 W m^{-1} K^{-1} at 300 K, whose value is ~43 % of that of pristine $CuFeS_2$.

Poster Presentation : **MAT.P-397**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Matrix composted nanoparticle inks for paper-based thermoelectric thermocouple using ballpoint pen printing

Eunjin Huh, Nayoon Pyun, So Jung Kim[1], Hyuckjin Lee, Oh-Sun Kwon*, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea
[1]*Biomedical Engineering , University of British Columbia, Canada*

Instead of complicated processes or expensive devices for current making electronics, we performed paper-based electronics using only one-step ballpoint pen printing technique to increase accessibility and lower cost. With two material inks, i.e. carbon nanotubes (CNTs) of less than 2 μm tube length and metallic silver nanoparticles (AgNPs) of less than 70 nm diameter, with viscosities 42 cP and 16 cP, respectively, the patterned thermocouple formed thermoelectric junction has been printed one paper smoothly. Morphological SEM images show that the ballpen printed material inks adhere well onto the surface of the paper with fine resolution and uniform thickness by rollerball pressing. Not only superiority in thermal conductivity and electrical properties, but CNT also showed a high thermoelectric effect. For AgNP/CNT coupling junction, the average Seebeck coefficient was $S = +8.62$ μV/K with varying in quadratic behavior in a range of 30 – 130 ℃. The Seebeck coefficient was varied by the deposition order on paper and the area of interfacial junction. We found that the overlay printing of AgNPs on CNTs showed the nanostructure-enhanced matrix formation establishing the increasing the contact area and so the phonon scattering than that of in opposite printing order and that it was nature due to novel structural difference of bead and tube of AgNP and CNT respectively.

Poster Presentation : **MAT.P-398**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Adsorptive removal of nitro- or sulfonate-containing dyes by a functional metal–organic framework: Quantitative contribution of hydrogen bonding

Md abul Hossain

Department of Chemistry, Kyungpook National University, Bangladesh

The removal of organic dyes from water is important from the perspective of sustainability. In this study, the adsorptive removal of four dyes having nitro or sulfonate groups was performed using highly porous metal–organic frameworks (MOFs, MIL101s) with or without further functionalization. In particular, a melamine-functionalized MOF (MIL101-Mela) was effective in the removal of martius yellow (MY), naphthol yellow S, orange G, and sunset yellow FCF. For example, the adsorbed quantity of MY over MIL101-Mela, even after the fourth recycle, was 6.9 times that over the fresh activated carbon. Moreover, MIL101-Mela showed higher adsorption capacity for the four studied dyes than previously reported any adsorbent. The adsorption results suggest the importance of the number of hydrogen donors and hydrogen acceptors in adsorbents and dyes, respectively, for improved performance in dye removal. Importantly, the mechanism of the dyes adsorption over the functionalized MIL101s is explained by the formation of six-membered rings between the studied MOFs and the dyes via hydrogen bonding. This work will pave the way toward the development of effective adsorbents for organics having high concentration of nitro or sulfonate groups. Keywords: Adsorption; dyes; hydrogen bond; metal–organic frameworks; six-membered ring

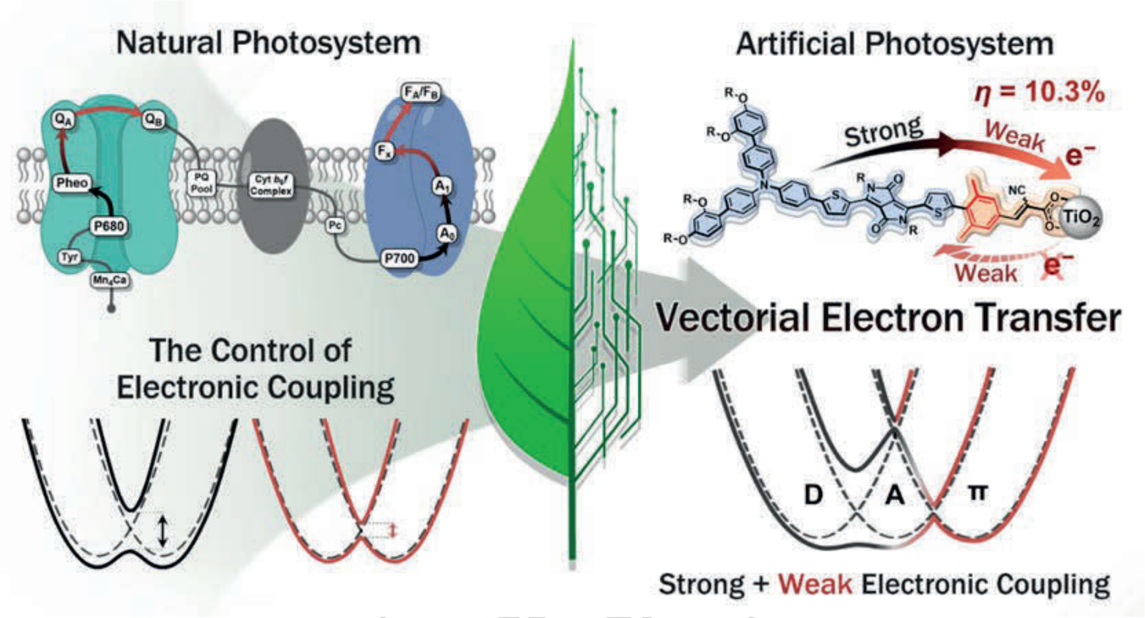
Poster Presentation : **MAT.P-399**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Molecular Design Strategy for Realizing Vectorial Electron Transfer in Photoelectrodes

Deok-Ho Roh, Tae-Hyuk Kwon*

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

Vectorial electron transfer, which is characteristic of natural photosystems and is driven by free-energy gradients and the control of electronic coupling, is essential for developing ideal artificial photosystems. Organic 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 molecular-design strategy for integrating strong (~600 cm−1) and relatively weak (310 cm−1) electronic coupling in a single sensitizer to realize vectorial electron transfer in dye-sensitized solar cells. Four sensitizers with donor–acceptor–π-spacer and anchoring group configurations (DD-DPP-Ph, DD-DPP-MP, DD-DPP-DMP, and bTPA-DPP-DMP) are developed, and the electronic coupling in these sensitizers is controlled by the π-spacers of varying steric hindrance. Femto-/nanosecond 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 to TiO2, which is attributed to strong electronic coupling between the donor and acceptor. The optimized sensitizer with integrated strong and relatively weak electronic coupling, bTPA-DPP-DMP, exhibits an improved photovoltaic performance of 10.3% power-conversion efficiency compared with the control sensitizer, DD-DPP-Ph.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P700
The Control of Electronic Coupling
Artificial Photosystem
η = 10.3%
Strong
Weak
e⁻
Weak
e⁻
TiO2
NC
Vectorial Electron Transfer
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π
Strong + Weak Electronic Coupling

Poster Presentation : **MAT.P-400**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Ni@N-Doped Carbon Shell as Ni-N-C Nanostructured Materials for Electrocatalytic Oxygen Evolution

<u>Juheon Han</u>, Minseon Choi, Yunseok Shin, Jinyoung Son, Hyeju Park, Sungjin Park[*]

Department of Chemistry, Inha University, Korea

The atomic-attached Ni species have attracted much attention to the replacement of high-precious metal catalysts for oxygen evolution reactions (OERs) due to their high activity. In this work, a new Ni-based core-shell material (Ni@Ni-NC) is produced through heat treatment of urea and NiCl2(H2O)6 mixtures. Microscopic characterizations shows that the old core-shell part is connected through a planar linker part. The core-shell section has layers of metallic Ni nanoparticles that are several tens of nanometers thick. Spectroscopy shows that the flat linker section and shell contain Ni-based species that are atomically attached to the N-doped carbon network (Ni-NC). Ni@Ni-NC exhibits excellent electrocatalyst OER performance with overpotentials of 371 mV and 1.51 V and superpotentials of commercial IrO2, respectively. Various control experiments have shown that well-dispersed Ni-NC species and core-shell structures play a pivotal role in improving electrocatalyst OER performance. The formation mechanisms of core-shell materials are studied using control samples generated using different heating time and density functional theory (DFT) calculations. The DFT calculation also proposes a dual-site OER mechanism for Ni-NC active species with significantly lower reaction barriers.

Poster Presentation : **MAT.P-401**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Photocatalytic degradation of organic dyes by CuO Nanoparticles supported on functionalized carbon nanotubes

Ji Dang Kim, Hyun Chul Choi*

Department of Chemistry, Chonnam National University, Korea

For solution to environmental problems, photocatalytic degradation using oxide-based photocatalysts is focus on organic pollutants in recent years. Among the photocatalysts, the advantages of copper oxide (CuO) are low toxicity, low cost, and physical and chemical stability. However, the applications of CuO nanoparticles remain limited by weakness in terms of their easy aggregation and the difficult separation from the product. To solve these limitations, we synthesized CuO decorated carbon nanotubes (CuO-CNT) composites by introducing thiol groups on surface of CNTs for enhance photocatalytic activity. The structure and elemental content of CuO-CNT nanocomposites were characterized by X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and transmission electron microscopy (TEM). In addition, the photocatalytic activities are examined with CuO-CNT using various organic dyes.

Poster Presentation : **MAT.P-402**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Na_3SbSe_4 based solid electrolytes for All-Solid-State Sodium Batteries

<u>Aarthi Uthayakumar</u>, Woon Bae Park[1,*]

Department of Advanced Components and Materials Engineering, Suncheon National University, Korea
[1]*Department of Printed Electronics Engineering, Suncheon National University, Korea*

Nowadays, the renewable and clean energy system becomes imperative due to the depletion of fossil sources and emission of harmful environmental pollution, but it fails to provide regular supply, since their source constraints with the time. The challenges posed by the intermittent renewable sources certainly require the energy storage system to ease the issue. Rechargeable batteries are an excellent alternative with the ability to store chemical energy and convert it into electrical energy with paramount efficiency. All-solid-state batteries replacing the liquid electrolyte with solids are in greater interest due to their enhanced stability, absence of leakage and flammability, and easy direct stacking. Sodium-ion batteries have attracted excessive attention due to their lower cost and higher availability compared to lithium-ion conductors. Thus, the high ionic conducting and electronically insulative electrolytes are of greater significance for All-solid-state sodium batteries. The cubic phase of Na3SbSe4 exhibits high ionic conductivity (~1 $mScm_{-1}$) due to the lower diffusion pathway connecting the tetrahedral and octahedral sites. It is interesting to explore the diffusion pathway by tuning the imperative factors such as the electronegativity, polarizability of the anions, and size of the sites. In this work, we report the synthesis and characterization of the fast Na-ion conductor, Na_3SbSe_4 with excellent ionic conductivity at room temperature, with dopant variants in the Se site. This compound will be a promising electrolyte for the all-solid-state sodium batteries.

Poster Presentation : **MAT.P-403**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Cost-effective Superionic Halide Solid Electrolytes for All-Solid-State Li-Ion Batteries

Seung-Tae Hong*, **Jaehee Won**[1]

Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Korea
[1]*Energy Science & Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

All-solid-state batteries (ASSBs), which have a low risk of explosion due to the use of a solid electrolyte that does not form dendrites, are attracting attention as a safe next-generation battery. The required conductivity as a solid electrolyte is about 10^{-4} S/cm. Recently, as many halide materials with lithium-ion conductivity of 10^{-4} S/cm or higher have been reported, the halides are being re-lightened. In addition, they are advantageous in comparison with oxides and sulfides due to their deformability, wide electrochemical stability window, and air stability. The Li_3MCl_6 family that has several Li sites in the lattice is the most well-known among the halides because many materials with high conductivity have been reported like Li_3YCl_6 (5.1×10^{-4} S/cm), Li_3ErCl_6 (3.3×10^{-4} S/cm), especially Li_3InCl_6 reached 1.4×10^{-3} S/cm. Cost-effective Li_2ZrCl_6 using Zr^{4+}, several times cheaper than M^{3+}, has also been reported to have acceptable conductivity. Here, based on previous research, an experiment was conducted to replace Zr^{4+} with In^{3+} to improve ionic conductivity. Li_2ZrCl_6, which has HCP structure, is changed to CCP structure through 2 phase mechanism as In^{3+} was substituted. The conductivity reached 0.8×mS/cm in the In^{3+} substituted sample, an improvement of 2.6 times compared to Li_2ZrCl_6. An ASSB using Li-In anode and NMC cathode exhibits good cycling stability up to 3.8 V at room temperature with a capacity of more than 100 mAh/g.

Poster Presentation : **MAT.P-404**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Anisotropic Gold Nanobipyramids Decorated with Anatase TiO_2 for NIR-triggerd Synergistic Photothermal and Photodynamic Cancer Therapy

Dohyub Jang, Dong Ha Kim[1,*]

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

UV-responsive anatase titania ($aTiO_2$) semiconductor has been considered as a promising photosensitizer due to their high photo-stability, non-toxicity, and cost-effectiveness. To achieve the extension of absorption range and introduce thermal modality, in recent years, incorporating $aTiO_2$ with plasmonic nanostructures with tunable localized surface plasmon resonance (LSPR) properties has been extensively developed. Previous reports of titania-coated gold nanoclusters have, however, been limited their properties with the aggregation and a clear morphological disruption of incorporated gold nanostructures during the hydrothermal steps required for the crystallization of the introduced TiO_2 phase. Herein, we introduce a novel strategy to decorate $aTiO_2$ onto gold nanobipyramids (Au NBP) at low temperature ranges. The resulting well-defined Au NBP/$aTiO_2$ core/shell structures maintained their initial morphology and sharp metal tips responsible for strong electric fields. Photo-catalytic activities of our core/shell nanostructures showcased the generation of reactive oxygen species under light illumination, demonstrating an injection of LSPR-induced hot electrons onto the $aTiO_2$ conduction band, resulting from the well-preserved sharp gold tip and clear monodispersity of our materials. *In vitro* and*In vivo* results further demonstrated the superior photothermal and photodynamic dual therapeutic effect. Our well-defined Au NBP/$aTiO_2$ core/shell structures may open up a new paradigm for the NIR responsive phototherapy.

Poster Presentation : **MAT.P-405**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

High thermoelectric performance of n-type $Bi_2Te_{2.7}Se_{0.3}$ by incorporating excess monovalent cations

Hyungseok Lee, Chung In[1,*]

Center for Correlated Electron Systems (IBS) and School of Chemical and Biological Engineering, Seoul National University, Korea

[1]*Center for Correlated Electron Systems (IBS) and School of Chemical and Biological Engineering, Seoul National Univerisity, Korea*

Bi_2Te_3 has been widely studied owing to its remarkable electrical transport properties and subsequent high thermoelectric (TE) performance. For commercial TE application of Bi_2Te_3-based system, it is required that TE properties of both p- and n-type materials be enhanced. However, there are few dopants to optimize electrical and thermal transport properties of n-type Bi_2Te_3 matrix, which results that development of n-type Bi_2Te_3-based system has been retarded compared to that of p-type Bi_2Te_3-based system. Here we report n-type Bi_2Te_3 system by incorporating excess monovalent cations. Excess monovalent cations not only substitute Bi site in matrix, but also intercalate van der Waals gap and interstitial sites in Bi_2Te_3 layers. Former substitution might modulate the band structure and latter intercalated cations can donate extra electrons. Both synergetic effects contribute to minimizing reduction in power factor of ~26.6 $\mu W\ cm^{-1}\ K^{-2}$ at 300 K. Moreover, these point defects from excess monovalent cations might soften heat-carrying phonon, which leads to decrease of lattice thermal conductivity down to ~0.22 $W\ m^{-1}\ K^{-1}$ at 400 K. Consequently, the peak TE figure of merit (ZT) of ~1.20 at 400 K is accomplished for nominal composition "$K_{0.6}Bi_2Te_{2.7}Se_{0.3}$".

Poster Presentation : **MAT.P-406**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis and Photophysical Properties of Light-Harvesting Gold Nanoclusters Fully Functionalized with Antenna Chromophores

Hongmei Xu, Kyunglim Pyo[1], SangMyeong Han, Dongil Lee[*]

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

The development of efficient light-harvesting systems is important to understand the key aspects of solar-energy conversion processes and to utilize them in various photonic applications. Here, atomically well-defined gold nanoclusters were synthesized as a new platform to fabricate artificial light-harvesting systems. An efficient amide coupling method is developed to synthesize water-soluble Au_{22} clusters fully protected with pyrene chromophores by taking advantage of their facile phase-transfer reaction. The synthesized Au_{22} clusters with densely packed 18 pyrene chromophores (Au_{22}–PyB_{18}) exhibit triple-emission in blue, green, and red wavelength regions arising respectively from pyrene monomer, pyrene excimer, and Au_{22} emission, producing bright white light emission together. The photoluminescence of Au_{22} is enhanced by more than tenfold, demonstrating that pyrenes at the periphery efficiently channel the absorbed energy to the luminescent Au_{22} at the center. Moreover, a combination of femtosecond transient absorption and anisotropy measurements provided a clear picture of energy transfer/migration processes occurring in Au_{22}–PyB_{18}. The structurally well-defined gold clusters exhibiting unique luminescent properties constitute a powerful model system to gain deeper understanding of the solar energy conversion processes. Further, the effective conjugation method developed for the preparation of densely functionalized gold clusters may have broad implications not only in photonic applications but also in other areas including biological imaging and drug delivery.

Poster Presentation : **MAT.P-407**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synergetic strategy of the surface polarity and crystal defect of conductive substrate to optimize electrocatalytic activity of metal nanocluster

Xiaoyan Jin, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

Hybridization with 2D nanosheets has attracted intense research interest because of its high efficacy in exploring high-performance hybrid catalyst materials. As an emerging conductive hybridization matrix, holey titanium oxynitride 2D nanosheet with nitrogen vacancies is synthesized by the ammonolysis of exfoliated titanate nanosheet due to the aliovalent substitution of divalent O^{2-} ion with trivalent N^{3-} ion. The nitrogen vacancies in holey titanium oxynitride nanosheet can act as efficient anchoring sites for Pt nanoclusters. The resulting strongly-coupled Pt-$TiN_{1-x}O_x$ nanohybrids commonly display excellent electrocatalyst performances for hydrogen evolution reaction (HER) with unusually high efficiency per Pt mass. The present study underscores that employing holey titanium oxynitride nanosheet as an immobilization matrix provides useful way of exploring atomically-dispersed metal electrocatalysts via enhanced interfacial chemical interaction.

Poster Presentation : **MAT.P-408**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Tunable structural colors of crystalline colloidal array of core-shell Iron oxide nanoparticles in non-polar medium

Jungmin Kim, Wonmok Lee[1,*]

Chemistry, Sejong University, Korea
[1]Department of Chemistry, Sejong University, Korea

Super-paramagnetic iron oxide nanoparticles (SPION) can be used as display material that respond to magnetic and electric fields.In this study, SPION@silica core-shell nanoparticles that form crystalline colloidal array (CCA) were synthesized by hydrothermal method, and the CCAs in polar solvent were confirmed to show reflective colors in the visible region.By using dispersing agent and charge control agent respectively, the CCAs showed structrual colors in non-polar solvents, and the color tuning was successfully carried out by magnetic field and electric field.

Poster Presentation : **MAT.P-409**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhancement of Thermoelectric Properties by Multiple Carrier Scattering by Superparamagnetism in Cu_2SnS_3

Sujin Kim, Sung-Jin Kim[1,*], Junphil Hwang[2]

Nano chemistry, Ewha Womans University, Korea
[1]*Department of Chemistry, Ewha Womans University, Korea*
[2]*Ewha Womans University, Korea*

Thermoelectric materials have attracted in recent decades due to their ability of reversible conversion between heat and electricity. The efficiency of thermoelectric devices can be evaluated by $zT=S^2\sigma T/\kappa$, S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature and κ is the thermal conductivity. The enhancement of zT is challenging due to their strong co-relation with Electrical conductivity and Seebeck coefficient. Therefore, improving the power factor is the most feasible strategy to enhance the efficiency of thermoelectric materials.In this work, we studied eco-friendly Cr-doped Cu_2SnS_3 material with $CuCrSnS_4$ nanoparticles. We found that doping Cr to Cu_2SnS_3 enhanced the carrier concentration $2.5\text{x}10^{20}$ cm^{-3} (Cr=0%) to $2.5\text{x}10^{20}$ cm^{-3} (Cr=20 %) and $CuCrSnS_4$ magnetic nanoparticles induced multiple scattering and it increased the Seebeck coefficient to 101.3 μV/K, resulting in a power factor increase from 1.12 to 6.67 $\mu W/cmK^2$.The $CuCrSnS_4$ were verified that second phase in Cu_2SnS_3 matrix by powder XRD patterns. The size of $CuCrSnS_4$ confirmed that 50 nm by the TEM analysis. The $CuCrSnS_4$ nanoparticles act as magnetic impurity in Cu_2SnS_3 matrix. As a result, it was confirmed that magnetic nanoparticles induced the multiple scattering, which is the great strategy for increasing power factor. Finally, the average zT value of Cr-doped- Cu_2SnS_3 with magnetic nanoparticles is the highest value of 0.8 at 723 K comparing with pristine zT of 0.08 at 723 K.

Poster Presentation : **MAT.P-410**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis and Electrochemical Characterization of Vanadium 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*

Calcium-ion batteries, compared to lithium-ion batteries, have the advantages of high theoretical capacity due to the high electric charge of calcium ions, low price due to abundant reserves, and safety. However, a suitable cathode material for calcium ion batteries has not been developed. Currently, transition metal phosphates having a Nasicon structure such as $NaV_2(PO_4)_3$ have been reported as a promising candidate for a calcium ion battery. Here we present a promising $VNb(PO_4)_3$ as a cathode material for calcium ion batteries. This material is synthesized by electrochemically extraction of Na ion from $NaVNb(PO_4)_3$, which is synthesized by solid state method. The crystal structure of the material analyzed by X-rat diffraction measurement and comprising elements ratio of the material analyzed by energy dispersive spectroscopy measurement confirms that $VNb(PO_4)_3$ was successfully synthesized. Cyclic voltammetry, galvanostatic, discharge-charge, X-ray diffraction and elemental analysis were performed to measure the electrochemical performance of the material as the calcium ion battery. Electrochemical experiment result shows an initial discharge capacity of 220 mAh/g using 0.5 M $Ca(ClO_4)_2$ in acetonitrile as the electrolyte. After X-ray diffraction and elemental analysis, it was confirmed that calcium ions were intercalated and deintercalated reversibly in the material during the charging and discharging process. The result demonstrates the discovery of promising new intercalation type host materials for Calcium-ion batteries.

Poster Presentation : **MAT.P-411**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Hierarchically Interconnected Porous Carbons from Metal-Organic Frameworks for Stretchable Ionogel-based Supercapacitors

InCheol Heo, Min Seok Kang[1], Won Cheol Yoo[2,*]

Department of Applied chemistry, Hanyang University, Korea
[1]*Department of Applied Chemistry, Hanyang University, Korea*
[2]*Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea*

In design principle of carbonaceous materials for ultrahigh-energy supercapacitors (SCs), hierarchically interconnected micro-/meso-/macroporous carbons (HICs) are of highly desirable; however, a facile means to produce HICs still remains a challenge. Herein, we report coarsening-induced preparation of HIC polyhedron derived from polymer-infiltrated metal-organic framework (MOF). HIC shows ultrahigh surface area (3064 m2/g) and superior capacitive properties compared to non-interconnected large mesoporous carbon and micro-/small mesoporous carbon, presenting excellent capacitance of 268.4 F/g with energy density of 149 Wh/kg comparable to the best values of ionic liquid-based SCs to date. Such outstanding capacitive properties can be ascribed to substantially expedited ion-transport via hierarchically interconnected large meso-/macropores, resulting in the maximum utilization of micropores of carbon electrode. Furthermore, stretchable HIC-based SCs that operated at 120% strain with a very high areal capacitance of 33 mF cm−2 and energy density of 0.041 mWh cm−2 were also demonstrated. Therefore, this facile strategy can be applicable to other types of MOF-derived HICs employed in high-performance SCs compatible with wearable electronic devices.

Poster Presentation : **MAT.P-412**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

V-doped $MoSe_2$ Nanosheets as Excellent Hydrogen Evolution Reaction Catalyst

Seungjae Lee, Ik Seon Kwon[1], In Hye Kwak[2], Doyeon Kim[1], Surjeet Chahal[3], Jeunghee Park[4,*]

ADVANCED MATERIAL CHEMISTRY, Korea University Sejong Campus, Korea
[1]*Advanced Materials Chemistry, Korea University, Korea*
[2]*Micro Device Engineering / Microdevices, Korea University, Korea*
[3]*Department of Advanced Materials Chemistry, Korea University, Sejong Campus, Korea*
[4]*Department of Materials Chemistry, Korea University, Korea*

Layered 2D transition metal dichalcogenides (TMDs) are regarded as promising catalysts for the hydrogen evolution reaction (HER), the cathodic half-reaction of water splitting ($2H_2O \rightarrow O_2 + 2H_2$). A valid strategy to improve the catalytic activity of TMDs is the use of dopants. In the present work, we successfully synthesized 2H phase V-doped $MoSe_2$nanosheets using a one-pot colloidal reaction. Atomic-resolution scanning transmission electron microscopy (STEM) was employed to identify the distributions of Mo, V, and Se elements, showing significant V and Se vacancies, which became the richest at 30-40% V doping. The V incorporation enhanced the electrocatalytic performance toward hydrogen evolution reaction (HER) in both 0.5 M H_2SO_4 and 1 M KOH. The Gibbs free energy along the pathway of HER indicates that this maximum performance is due to the high concentration of active V and Se vacancy sites.

Poster Presentation : **MAT.P-413**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Phase Transition of $Mo_{1-x}V_xSe_2$ Alloy Nanosheets with Rich V-Se Vacancies

In Hye Kwak, Ik Seon Kwon[1], Doyeon Kim[1], Seungjae Lee[2], Surjeet Chahal[3], Jeunghee Park[4,*]

Micro Device Engineering / Microdevices, Korea University, Korea
[1] *Advanced Materials Chemistry, Korea University, Korea*
[2] *ADVANCED MATERIAL CHEMISTRY, Korea University Sejong Campus, Korea*
[3] *Department of Advanced Materials Chemistry, Korea University, Sejong Campus, Korea*
[4] *Department of Materials Chemistry, Korea University, Korea*

Alloys of transition metal dichalcogenide can display unique phase evolution because of their two-dimensional structures. Herein, we report the colloidal synthesis of $Mo_{1-x}V_xSe_2$ alloy nanosheets with full composition tuning. Alloying led to a phase transition at x = 0.7 between the semiconducting 2H phase $MoSe_2$ and the metallic 1T phase VSe_2. Atomic-resolution high-angle annular dark-field scanning transmission spectroscopy revealed that the V vacancies increase up to 10% as x approaches 0.5. The Se vacancies are preferentially formed adjacent to the V atoms, and their concentration reaches a maximum of 13% at x = 0.4. The sum of V and Se vacancies became the richest in the 2H phase at x = 0.3–0.5. Extensive spin-polarized density functional theory calculations consistently predicted the 2H-to-1T phase transition at x = 0.7, in agreement with the experimental results. It also successfully predicted the 2H-to-1T phase transition as x increased to 0.7. The vacancy formation energy showed that the alloying favorably produced V and Se vacancies that aggregated in a cooperative manner. These alloy phase nanosheets would provide a unique platform for exploring the physical and chemical properties upon phase tuning.

Poster Presentation : **MAT.P-414**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effects of cerium on Ni-based catalysts for dry reforming of methane

Jung-ho Lee, Su Jin Kim[1], Jae Ik Lee[1], Ji Man Kim*

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

The dry reforming of methane (DRM; $\mathrm{CO2} + \mathrm{CH4} \rightarrow 2\mathrm{CO} + 2\mathrm{H2}$) is attracting attention as a reaction to generate valuable synthesis gas using greenhouse gases, as an increase in concern for reduction and utilization of greenhouse gases. Nickel is most widely used as a catalyst for reforming, but the high reaction temperature of DRM causes aggregation of the catalysts and severe coke formation leading to deactivation. In this study, we prevented the sintering and coking by impregnating Ni and Ce nanoparticles into the mesoporous silica support. Cerium can increase the dispersion of Ni nanoparticles and stabilize catalyst during the reaction. The dispersion of the active site after thermal activation as well as the catalytic activity and stability of the catalyst after reduction will be presented.The synthesized catalytic properties were analyzed by X-ray diffraction (XRD), nitrogen adsorption and desorption isotherms, scanning electron microscope (SEM), transmission electron microscope (TEM), and temperature programmed reduction (TPR).

Poster Presentation : **MAT.P-415**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Defect Diamond-like Structure Semiconductors 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*

Solid-state electrolytes have emerged as a form of new high-capacity Li-ion batterires. Solid electrolytes do not use organic liquid electrolytes and volatile substances, which have the advantage of being safe from the risk of liquid leakage or explosion. In addition, it can be produced in various shapes and in the case of polymer solid-state electrolytes, it can be made of flexible materials, so it is easy to manufacture. However, since it has low ionic conductivity, research on materials and materials is needed to increase conductivity.In this study, we select a quaternary diamond-like structure(DLS) compounds with defect as a solid-state electrolyte which expected to have high lithium ion conductivity. For DLSs with cation defects, $LiZn(II)P(V)S_4$ research was preceded by Naoki Suzuki, and the ionic conductivity $\sigma_{25^\circ C}$ of $LiZnPS_4$ is ~10^{-8}Scm^{-1}. Based on this material, $Li_{1+2x}Zn_{1-x}PS_4$ structure was designed by substituting Li to the Zn(II) position and vacancy to have more Li ions in the structure, thereby increasing the ionic conductivity $\sigma_{25^\circ C}$ to 2.6×10^{-4}Scm^{-1}. We synthesized $LiM(III)M'(IV)S_4$ structure expected tetragonal structure with cation defect sites, and and these compound are expected bcc anion framework which could induce high Li-ion conductivity. $LiM(III)M'(IV)S_4$ compounds are analyzed the structural characteristics using PXRD and Rietveld refinement. The Li ion conductivity is measured by electrochemical impedance spectroscopy(EIS).

Poster Presentation : **MAT.P-416**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication of Ecofriendly Transparent Nanofibrous Sheet Containing Nanocellulose Extracted from Tunicate

Jimo Yang, Seonho Choi, Sang Eun Hong, Kuk Ro Yoon*

Department of Chemistry, Hannam University, Korea

Electrospinning has been extensively explored as it is recognized as an effective technique for the fabrication of polymeric, ceramic and hybrid nanofibers possessing high specific surface area, porosity and flexibility. Also, various electrospun nanofibers, polymeric nanofibers are widely used materials for conventional and high technology applications such as filtration, textile, scaffold, and wound dressing materials. Among different celluloses in green materials, nanocellulose extracted from tunicate (TCNF) have many characteristics such as high crystallinity, good thermal stability, and excellent mechanical properties. Which is quietly facile material for next-generation. In this work, transparent nanofibrous sheet was fabricated from tunicate nanocellulose with electrospinning and dipping method in water. The physicochemical properties were obtained by FE-SEM, XRD, FTIR, TGA and mechanical properties.

Poster Presentation : **MAT.P-417**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

4H-2H-1T Phase Coexistence of $Nb_{1-x}V_xSe_2$ Alloy Nanosheets to Enhance Catalytic Activity Toward Hydrogen Evolution Reaction

<u>Ik Seon Kwon</u>, In Hye Kwak[1], Doyeon Kim, Seungjae Lee[2], Surjeet Chahal[3], Jeunghee Park[*]

Advanced Materials Chemistry, Korea University, Korea
[1]*Micro Device Engineering / Microdevices, Korea University, Korea*
[2]*Advanced Materials Chemistry, Korea University Sejong Campus, Korea*
[3]*Advanced Materials Chemistry, Korea University, Sejong Campus, Korea*

Phase transition of transition metal dichalcogenide can open the possibility for many novel applications and architectures. Herein, we report the colloidal synthesis of $Nb_{1-x}V_xSe_2$ alloy nanosheets with full composition tuning. Phase conversion from the $NbSe_2$ to the VSe_2 occurs $x = 0.1 \sim 0.3$, where three phases coexist, accompanying the morphology evolution from a flower-like particle to a coin shape disk. It produced significant Se vacancies, which became the richest at $x = 0.2$. Extensive spin-polarized density functional theory calculations consistently predicted that the (4H, 2H)-to-1T phase transition occurs at $x = 0.3$ but shifts closely to $x = 0$ in the presence of Se vacancies, in agreement with the experimental results. The vacancy formation energy supports the favorable formation of vacancies in the 1H-1T phase domain boundaries. Alloying in the 1T phase enhanced the electrocatalytic performance toward hydrogen evolution reaction (HER) at $x = 0.2$ in both 0.5 M H_2SO_4 and 1 M KOH electrolytes. The Gibbs free energy along the pathway of HER indicates that this maximum performance is due to the highest concentration of active V and Se vacancy sites at the phase conversion composition.

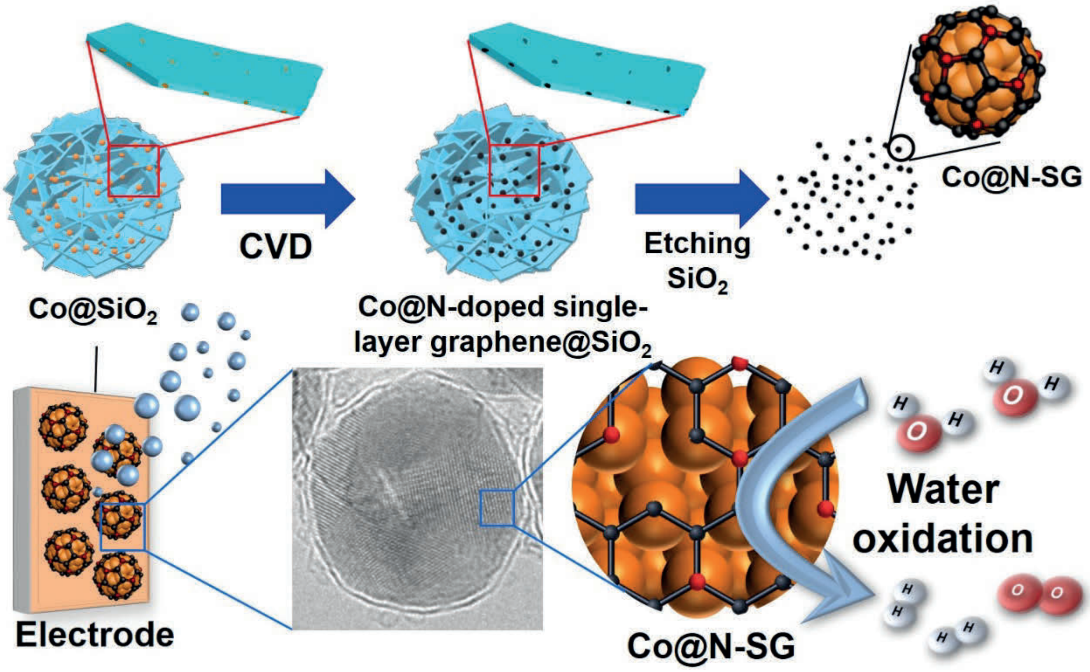
Poster Presentation : **MAT.P-418**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Controllable synthesis of single-layer graphene over cobalt nanoparticles and insight into active sites for efficient oxygen evolution

Gisang Park, Jong-Sung Yu*

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

Controllable synthesis of graphene-coated metal nanoparticles (NPs) presents a major challenge when considering the practical application of these catalysts. Herein, we use silica as a radical sieve to grow graphene over cobalt NPs via chemical vapor deposition. As-prepared single-layer graphene-coated cobalt NPs with and without N doping (Co@N-SG and Co@SG) exhibit noticeable oxygen evolution reaction (OER) activity. Furthermore, a magnet-assisted binder-free Co@N-SG electrode illustrates much improved OER activity and stability over conventional binder-assisted counterparts, suggesting this as an effective way to overcome the recognized issues of high electron transfer resistance and poor adhesion of binder-based electrodes in practical applications. Interestingly, the graphene shell possesses varying defects and major OER benefitting active sites are found around said defects in the shell, while separately isolated Co@SG with a defect-free shell, despite exhibiting a slightly lower initial activity, illustrates a much-improved durable OER performance. The underlying Co affects the electron density of the graphene shell through dipole interaction and the electron density is optimized for adsorption of reaction intermediates, hence accelerating OER performance.


CVD
Etching
SiO_2
Co@N-SG
Co@SiO_2
Co@N-doped single-
layer graphene@SiO_2
Electrode
Water
oxidation
Co@N-SG
H
O
H
O

Poster Presentation : **MAT.P-419**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Phase Transition of Polytypic Ga_2S_3 Nanowires and Their High Performance in UV Photodetection

Doyeon Kim, Surjeet Chahal[1], Ik Seon Kwon, In Hye Kwak[2], Seung Jae Lee[3], Jeunghee Park[4,*]

Advanced Materials Chemistry, Korea University, Korea
[1]*Department of Advanced Materials Chemistry, Korea University, Sejong Campus, Korea*
[2]*Micro Device Engineering / Microdevices, Korea University, Korea*
[3]*Department of Chemistry, Jeonbuk National University, Korea*
[4]*Department of Materials Chemistry, Korea University, Korea*

Polytypism of semiconductor nanostructures is of paramount importance for many promising applications in high-performance nanodevices. We report successful chemical vapor deposition synthesis of Ga_2S_3 nanowires (NWs) that show a phase transition of monoclinic (M) -> hexagonal (H) -> wurtzite (W) -> zinc blende (C) simply by lowering the growth temperature from 850 to 600 °C. At the highest temperature, single-crystalline NWs were grown in the thermodynamically stable M phase. The H phase exhibited 1.8-nm periodic superlattice structures consisting of the three rotational variants of the M phase along the growth direction ([001]M = [0001]H/W). At even lower growth temperatures, the W and C phases sequentially became the major ones with different growth directions ([01(_)10]W = [112]C) and [1(_)210]W = [110]C). The four phases mentioned above shared the same crystallographic axis within the NWs, producing unique core-shell structures to illustrate the phase evolution. Photodetector devices based on the p-type M-phase Ga_2S_3 NW showed excellent photoresponsivity (spectral responsivity: 1.8x 10^4) A W^{-1}).

Poster Presentation : **MAT.P-420**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication of AAO-based Heterodimer Nanoparticle Pea-Pod Nanostructures for SERS Applications

Jung-a Lee

chemistry, Gachon University Global Campus, Korea

Many studies have been conducted to compare optical properties different from those present as a single particle when two or more metal nanoparticles are adjacent. In this study, two metal nanoparticles were placed parallel to each other in an anodic aluminium oxide(AAO) substrate to create a highly uniform SERS substrate that forms a hot spot. The particles used in the experiment were Au and Ag nanoparticles, commonly known as plasmon materials. The SERS effect of the constructed substrate was measured by Raman spectroscopy to examine the differences. We found that the SERS signal of the substrate with two Heterodimers inserted was higher than that of the manufactured monomer substrate. As expected, AgNPs dimer substrate showed higher SERS signal than the AuNPs dimer substrate. Since the substrate can be made of nanoparticles with different plasmonic properties, it is expected that we can utilize novel SERS substrates by creating various different metal pea-pod structures.

Poster Presentation : **MAT.P-421**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication and Characterization of Poly(dimethyl sulfoxide-co-acrylic acid) (PDMSO-AA) Nanofibers for Surface Wettability Controlled: Synthesis of PDMSO-AA using Steglich Esterification

Seonho Choi, Sang Eun Hong, Kuk Ro Yoon[*]

Department of Chemistry, Hannam University, Korea

Dimethyl sulfoxide (DMSO) was a widely used solvent in biological, chemicals, that often DMSO helped medicines passed the skin barrier, and can affect proteins, fat, and carbohydrate in the body. Recently, the synthesized sulfoxide-containing polymer has been studying inspired by the physicochemical properties of DMSO, such as its excellent biocompatibility, negligible cytotoxicity, and super hydrophilic. In this study, we synthesized sulfoxide-functionalized polymer, and the fabricated PDMSO-AA nanofibers mimic the properties of DMSO. We analyzed the chemical properties of PDMSO-AA by FT-IR, UV-vis, 1H-NMR, TGA, DSC, and GPC. Also, the physical properties of PDMSO-AA nanofibers were improved mechanical strength (stress is 9 MPa, strain is 30 %) than PAA nanofibers, impressively PDMSO-AA nanofibers have highly hydrophilic properties like a DMSO from water contact angles. We expected to PDMSO-AA nanofibers may find applications for biomaterials like a wound dressing, transdermal patch, and fast drug delivery materials for skin and oral.

Poster Presentation : **MAT.P-422**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Cerium oxide based photocatalysts with controlled morphology and vacancy defects

Surjeet Chahal*, **Ik Seon Kwon**[1], **In Hye Kwak**[2], **Doyeon Kim**[1], **Seungjae Lee**[3], **Jeunghee Park**[4]

Department of Advanced Materials Chemistry, Korea University, Sejong Campus, India
[1]*Advanced Materials Chemistry, Korea University, Korea*
[2]*Micro Device Engineering / Microdevices, Korea University, Korea*
[3]*ADVANCED MATERIAL CHEMISTRY, Korea University Sejong Campus, Korea*
[4]*Department of Materials Chemistry, Korea University, Korea*

Cerium oxide nanostructured materials with different morphologies (nanosphere, microsphere, and spindle-shape composed of nanorods) have been synthesized using sol-gel and modified hydrothermal methods. The electronic properties were explored using Raman and X-ray photoelectron spectroscopy (XPS) to depict the defects in the lattice. Oxygen vacancies (VO) in CeO_2 lattice played the vital role in deciding their properties and were controlled by doping of trivalent (La^{3+}, Y^{3+}, Er^{3+} and Sm^{3+})/divalent (Mg^{2+}) metal ions in lattice. Room temperature ferromagnetic (RTFM) behavior was depicted in cerium oxide that strongly depends on the lattice defects and morphology of the nanomaterials. The synthesized nanomaterials have been studied to seek enhancement in the photocatalytic and magnetic properties for their use in photocatalysis and spintronic devices. Further, composites of cerium oxide nanoparticles with multi-walled carbon nanotubes (MWCNTs) and graphene oxide have been fabricated with enhanced photocatalytic activity towards organic pollutants.

Poster Presentation : **MAT.P-423**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Halogenated Low Bandgap Polymer Donor for Semi-Transparent Organic Solar Cells (ST-OSCs)

Hyemin Bae, Hyosung Choi[1,*]

Advanced Materials Division, Korea Research Institute of Chemical Technology, Korea
[1]Department of Chemistry, Hanyang University, Korea

Halogenated Low Bandgap Polymer Donor for Semi-Transparent Organic Solar Cells (ST-OSCs)Abstract: Semi-Transparent organic photovoltaics (ST-OPVs) have attracted significant attention for building-integrated photovoltaics (BIPV) and smart window technologies. While the various low-band gap non-fullerene acceptors were developed to realize the highly efficient organic photovoltaics (OPVs), polymeric donors for harvesting the near-infrared (NIR) were rarely reported. However, in order to construct the ST-OPVs' configurations, both the polymeric donors and acceptors are required to absorb NIR light, not visible region. In this work, halogenated BD-F and BD-Cl are synthesized by modifying BD-H which is well known as PBDTT-DPP that absorbs NIR light primarily. Among them, as expected, BD-Cl:Y6 shows the highest VOC and FF because of downshifted energy level of BD-Cl and balanced morphology. An opaque device based on BD-Cl:Y6 provides a power conversion efficiency (PCE) of 5.62%. When the blended layer is applied to semi-transparent solar cells, the PCE of 3.69% and AVT of 35.1% are achieved. This approach can be contributed to enhancing potential of semi-transparent solar cells.

Poster Presentation : **MAT.P-424**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Preparation and Characterization of Collagen and Lecithin Contained Starch Scaffold with Improved Biocompatibility

Mi Jeong Son, Seonho Choi, Sang Eun Hong, Kuk Ro Yoon*

Department of Chemistry, Hannam University, Korea

Starch is a natural polymer composed of glucose units linked by α-(1-4) glycosidic bonds. It is biocompatible and biodegradable as used in biomaterials. However, limitations such as water sensitivity and poor barrier properties at high moisture concentrations as a scaffold. To overcome these limitations, amphipathic lecithin reduces solubility, and collagen regulates cell attachment, proliferation, and differentiation, which were blended to prepare nanofibers by electrospinning. The morphology of the nanofiber was confirmed by a Field emission-Scanning electron microscope (FE-SEM), and the physicochemical properties are identified by Fourier transform-Infrared spectroscopy (FT-IR (ATR mode)), Tensile strength, Contact angle, Thermogravimetric analysis (TGA), Differential scanning calorimetry (DSC), degradability, cell proliferation assay, and fluorescence microscope. Interestingly, thermal stability was improved by hydrogen bonding between starch and collagen. Also, water-insoluble starch nanofibers were prepared by improving water stability due to the zwitterion of lecithin. As a result, starch nanofibers containing collagen and lecithin have improved biocompatibility and mechanical properties, and are expected to be applied to tissue engineering.

Poster Presentation : **MAT.P-425**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced Hydrogen Evolution Reaction Catalysis by Ni-Co Bimetallic Metal Organic Frameworks/Carbon Nanotubes Composites

Min Sung, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

Hydrogen has been attracting attention as a renewable energy alternative for fossil fuels due to recent environmental and climate issues. Especially, hydrogen production from water splitting reaction has been considered as a potentially clean process without forming waste compared to conventional gas-reforming processes. However, the slow-kinetics of water splitting is a huddle to achieve high efficiency, therefore, the development of electrocatalysts to overcome the kinetic issue is very important. In this research, Ni-Co based bimetallic metal-organic frameworks (BMOFs)/CNT composites were synthesized using hydrothermal method and applied as a HER catalysts. To optimize electrocatalytic performances, Ni-Co BMOFs with various composition and annealing temperature have been compared, and the best catalysts shows -163 mV overpotential and 118 mV/dec at -10 mA/cm^2. Electrocatalytic performance changes depending on the BMOF distribution on CNT, size of metal particles, and defects if CNT will be discussed.

Poster Presentation : **MAT.P-426**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication of Acetalated-Dextran Nanofibers by Solution Blow Spinning for Hemostasis Effect

Mi Jin Park, Seonho Choi, Sang Eun Hong, Kuk Ro Yoon*

Department of Chemistry, Hannam University, Korea

Acetalated-Dextran (Ac-Dex) was made hydrophobic by acetalation of Dextran, a hydrophilic polysaccharide mainly composed of α- (1 → 6) bonds. Also, the used biomaterial because of no change in pH due to degradation products. Solution blow spinning (SBS) requires simple apparatus, utilizing only an airbrush and polymer solution. That is possible to a quickly large area of formed nanofiber mats, without pressure nanofibers on soft tissues such as livers. In this study, fabricated large area Ac-Dex nanofibers that mimicked the fibrin by SBS. When nanofiber mats direct deposition to the bleeding site, it showed stopped bleeding. And Ac-Dex nanofiber mats were confirmed through the MTT results that the cytotoxicity was low. Particularly, which morphology of nanofiber mat has been maintained for 72 hours in PBS condition was due to acetalation of dextran. At the result, fabricated Ac-Dex nanofiber through SBS is expected to apply to a hemostatic system that can short-time control excessive bleeding.

Poster Presentation : **MAT.P-427**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Enhancing n-type thermoelectric performances of polycrystalline SnSe via PbSe alloying and Cadmium doping

Sejin Byun, Chung In[*]

Center for Correlated Electron System (IBS) and School of Chemical & Biological Engineering, Seoul National University, Korea

Thermoelectric technology enables direct and reversible transition between heat and electric energy, thereby a promising means of sustainable power generation via waste heat harvesting. Recently, single crystal SnSe materials received great attention for their high thermoelectric performance over temperature range of 773− 923 K mainly due to highly anisotropic crystal structure. In addition, SnSe is composed of less toxic and earth abundant elements, suitable for economical thermoelectric power generation systems. Despite these advantages, extensive use of single crystal SnSe samples are limited because they are not easy to synthesize and have poor mechanical properties. Very recently, thermoelectric performance of p-type polycrystalline SnSe materials showed even higher values than those of single crystal SnSe samples. However, the development of n-type polycrystalline SnSe is still challenging due to its intrinsic p-type nature. Here we present high performance n-type polycrystalline SnSe system by PbSe alloying and cadmium doping. By optimizing alloying and doping rate, we optimized electron carrier concentration of n-type SnSe system, which improves power factors significantly. It also reduces thermal conductivities due to point defect scattering of heat-carrying phonon simultaneously. As a result, a high thermoelectric figure of merit of ~1.7 at 873 K is achieved for the optimized samples.

Poster Presentation : **MAT.P-428**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Synthesis of NiCo Layered double hydroxide with polyethylene glycol template

Jing Xie, Jae-Min Oh[1,*]

Energy and Materials Engineering, Dongguk University, Korea

[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*

We have successfully prepared NiCo based layered double hydroxides (LDH) utilizing polyethylene glycol (PEG) as a structure-directing template. The NiCo-LDH was prepared by coprecipitation Co(II)/Ni(II) with NaOH solution under the existence of PEG, and was characterized with X-ray diffraction (XRD), inductively coupled plasma - optical emission spectrometry (ICP-OES), nitrogen adsorption-desorption isotherm, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The XRD patterns indicated that the prepared LDH had higher crystallinity compared with the previously reported NiCo-LDH without PEG template. The ICP-OES showed the Ni/Co ratio in the sample was 1/3 which was lower than the nominal ratio of 1/2, implying that Co was less stabilized in this templated synthesis. The nitrogen adsorption-desorption isotherm results presented NiCo-LDH had a fairly high surface specific area of 76 m2/g with slit-shaped pores. The result exhibited that the PEG templated directed LDH particle growth into a three-dimensional structure, which was also visualized as a flower-like structure in SEM measurement. The XPS results revealed the coexistence of Co(II) and Co(III) in LDH, suggesting the partial oxidation of Co(II) during LDH crystal growth. It was expected that the PEG acted as coordination sites for metal cations (Ni or Co) to facilitate structural development of LDH layers which were interconnected in a three-dimensional flower-like structure.

Poster Presentation : **MAT.P-429**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Co(II) incorporation into drug-layered double hydroxide hybrid with cancer targeting ligands on particle surface

Chandrabose Vidya, Jae-Min Oh[1,*]

Energy And Materials Engineering, Dongguk University, Korea
[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Co(II) incorporation into drug-layered double hydroxide hybrid with cancer targeting ligands on particle surface Chandrabose Vidya, Jae Min Oh Department of Energy And Materials Engineering, Dongguk University, Seoul, 04620, Republic of Korea.Theranostics nanomedicine is a novel and the most expanding approach that involves the combination of diagnostics and therapeutics for the safe and targeted drug delivery. In this work, theranostic nanomedicine was prepared based on the hybrids of anticancer drug, methotrexate (MTX) and two-dimensional delivery carrier, layered double hydroxide (LDH). The drug containing MgAl-LDH (MTX-LDH) was synthesized by co-precipitation method and the surface of particles was modified with folic acid (FA) ligand directly or with the existence of hexamethyldiamine (HDA) spacer between particle and FA. The synthesis involves a series of coupling reactions, initially starting from the silicon coupling agent, 3-amino propyl silane (APS). The FA moiety was either directly attached to amine terminal of APS or linked with APS through HDA and 1,4-butane diisothiocyanate moiety by thiourea formation. Then the materials was reacted with aqueous Co(II) solution at 150 degrees of hydrothermal condition to facilitate incorporation of Co(II) into LDH lattice. All the materials before and after surface modification were characterized by X-ray diffractometry, scanning electron microscopy, X-ray adsorption spectroscopy, and Fourier-transform infrared spectroscopy and Fourier-transform extended Xray absorption fine structure (FT-EXAFS) spectra. The results confirmed that Co(II) was successfully incorporated in to the MTX-LDH hybrids even with targeting ligand on the particle surface. The hydrothermal reaction did not alter the crystalline phase, size or particle morphology, suggesting that the radioisotope metal such as Co-57 can be incorporated to drug-LDH hybrids with cancer targeting moiety.

Poster Presentation : **MAT.P-430**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Transparent luminescent solar concentrator assisted by energy transfer between quantum dots and hexarhenium cluster dyes

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 concentrator (LSC) is a solar-light harvesting device that concentrates sun light on a photovoltaic cell placed at the edge of an LSC panel to convert it into electricity. The nano-sized inorganic–organic cluster complex $(dMDAEMA)_4[Re_6S_8(NCS)_6]$ (this refers to RMC where dMDAEMA is 2-dimethyl amino ethyl methacrylate) is a promising candidate for LSC luminophores due to its downshifted broad photoluminescence suitable for photovoltaic cells. However, the low photoluminescent quantum yield (PLQY) of RMC limits the performance. Here, zinc-doped CuGaS/ZnS core/shell quantum dots (ZQD) were used as energy transferring donor with high PLQY to enhance the performance of the LSC. The two metal chalcogenide luminophores, RMC and ZQD, are chemically suitable for dispersion in an amphiphilic polymer matrix, resulting in a transparent waveguide with suppressed reabsorption and extended harvesting coverage of the solar spectrum. We achieved an ηopt of 3.47% and a PCE of 1.23% while maintaining greater than 80% transparency in the visible range. The performance of this device was also evaluated by measuring the current density over distance and proved to be more stable when the two dyes were used together. The high performance of this dual-dye LSC with suppressed reabsorption, and scattering losses is not only due to uniform dispersion of dyes in a polymer matrix, but also energy transfer from ZQD to RMC. This report suggests a new possibility for promising various multi-dye LSCs for use in building-integrated photovoltaic (BIPV) windows.

Poster Presentation : **MAT.P-431**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Laser induced Co-Ni/rGO composites for enhanced Micro-Supercapacitor

Jae Ryeol Jeong, Dakyung Jung, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

Development of facile fabrication method of flexible micro-supercapacitor (MSC) attracts much attention due to public interests to wearable electronic device. Recently, the trend of development for MSCs has large interests to smaller, thinner, lighter, more flexible and high energy density. Among the various energy storage devices, MSCs are promising candidate due to high-power capabilities, long cyclic life, and rapid charge and discharge rates. In this study, controlled growth of Co-Ni/rGO composites on flexible substrate is successfully fabricated using laser-scribing method. Patterned Co-Ni/rGO MSCs show excellent electric conductivity compared to pristine rGO and this advantage could be contributed to increase power density. Also, pseudocapacitic behavior of Co-Ni increase energy density of rGO MSC in the same volume.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **MAT.P-432**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced catalytic performance of bimetallic dual ligand MOF for oxygen evolution reaction

Jungjun Lee, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

Accelerating of global warming due to the increase the greenhouse gas releasing was continuously raised problems. To prevent the accelerating of global warming, numbers of researchers study about the renewable energies (i.e., hydrogen, solar and wind energy) to reduce carbon dioxide (CO2) which is representative greenhouse gas. Among them, hydrogen (H2) energy is one of the most attractive candidate and it can be produced to water electrolysis. Oxygen evolution reaction (OER) is key reaction for water splitting due to their sluggish kinetics. Herein, we synthesized hetero metal and ligand introduced metal organic framework (MOF) and evaluated the electrochemical properties for OER. In SEM images, hetero components introduced MOF appeared slightly different morphology. Bimetallic dual ligand MOF is well matched to pristine Ni-based MOF in XRD pattern. As synthesized MOF exhibited the decreased overpotential, charge transfer resistance (Rct) and Tafel slope. Furthermore, modified MOF showed the higher electrochemical active surface area (ECSA) and turnover frequency (TOF) values.

Poster Presentation : **MAT.P-433**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced Oxygen Evolution Reaction Catalysis by Fe-doped NiSe

Sun Mi Kim, **Min Hyung Lee**[*]

Department of Applied Chemistry, Kyung Hee University, Korea

Developing highly efficient, stable, and low-cost electrocatalysts for oxygen evolution reaction (OER) is important issue to realize cost-economic hydrogen production using electrolysis of water. Most reported OER catalysts based on transition metals exhibit high overpotential due to sluggish kinetics of OER processes. To overcome this issue, we develop simple synthetic process of Ni-Se based catalysts with unique electronic structure. The XRD results revealed that synthesized materials show hexagonal NiSe, and hexagonal Ni_3Se_2 phases. Electrocatalytic performance of Fe-NiSe deposited on a Ni foam (designated as Fe-NiSe/NF) was improved significantly in alkaline solution with overpotential of 239 mV at 100 mA cm^{-2} and Tafel slope of 60.6 mV dec^{-1}. In addition, chronoamperometry shows that Fe-NiSe/NF remain stable over 100 hours operation in 1 M KOH. According to thorough experimental investigation, we concluded that enhanced conductivity and increased active sites by doping Fe on NiSe are the key factor of the enhanced OER performances.

Poster Presentation : **MAT.P-434**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced Electrochemical Performance of Self-Assembled NiFe LDH@rGO

Hye Yeon Yoo, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

Due to recent environmental issues, hydrogen energy has attracted great attention as a clean and sustainable energy source. Currently, over 95% of hydrogen production relies on conventional gas reforming processes, which produce CO_2 and CO waste during processes. Therefore, electrochemical water electrolysis is attractive as an alternative method to produce hydrogen at ambient condition without environmental wastes. However, industrial level production of hydrogen using water electrolysis is still limited by slow kinetics of oxygen evolution reaction (OER), which is a half-reaction of water electrolysis. Therefore, a lot of effort has been made to develop highly efficient transition metal-based electrocatalysts to enhance the kinetics of OER. Layered double hydroxide (LDH) is an attractive material for OER catalyst, since it can simply introduce bimetals and can stabilize intermediates in between layers. In this poster, a NiFe LDH@rGO catalyst was synthesized by self-assembly, and it showed lower overpotential (220 mV@10 mA/cm^2) and Tafel slope (67.4 mV/dec) compared to the pristine NiFe LDH by improved conductivity.

Poster Presentation : **MAT.P-435**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Surface structure investigation of colloidal quantum dot nanoparticle by advanced transmission electron microscopy

Hayeon Baek, **Sungsu Kang**[1], **Jungwon Park**[1,*]

Chemical Biological Engineering, Seoul National University, Korea
[1]*Chemical and Biological Engineering, Seoul National University, Korea*

Colloidal quantum dot (QD) is a promising candidate for the next-generation light emitting device. However, QD typically suffers from suppression of the luminescence properties, as the formation of surface defects mainly originates from high oxophilicity of QD generates trap sites for charge carriers. Therefore, it is important to investigate surface structure of quantum dot nanoparticle for the development of stable and highly luminescence QDs. Here, to investigate surface chemistry of QD nanoparticle, we developed analytical methods based on high-resolution transmission electron microscopy (TEM). Surface structures of QDs are investigated at an atomic level using aberration-corrected TEM of QDs on a graphene substrate and a direct electron detector which enables the use of low electron fluency. In addition, we developed graphene liquid cell for in situ observation of fluctuations in QD surface structures in liquid. Our novel approaches for examining the QD surface structure will be applied to other systems of nanomaterials which require understanding of atomic structures.

Poster Presentation : **MAT.P-436**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Integrated Material and Process Investigation of Metal-organic Frameworks Database for Energy-efficient SF_6/N_2 Separation

Jaehoon Cha, Yongchul Chung*

School of Chemical Engineering, Pusan National University, Korea

The high dielectric strength of SF_6 makes the gas useful in gas-insulated switchgear, where SF_6 is typically mixed with relatively cheap N_2. However, SF_6 has been identified as one of the main greenhouse gases due to its high global warming potential (GWP: 22,800 - 23,900). In this work, we proposed multi-scale screening, which employs both molecular and process-level methods, to identify high-performing MOFs for energy efficient separation of SF_6 and N_2 mixture. Grand canonical Monte Carlo (GCMC) simulations were combined with ideal adsorption process simulation to computationally screen 2,890 metal-organic frameworks (MOFs) for adsorptive separation of SF_6/N_2. More than 150 high-performing MOFs were identified based on the GCMC simulations at the pressure and vacuum swing conditions, and subsequently evaluated using the ideal adsorption process simulation. 78 out of 86 MOFs selected for the VSA conditions were able to achieve the 90 % target purity level of SF_6, but 62 top-performing MOFs selected for the PSA condition could not reach the purity level with a single train PSA configuration. Cascade PSA configuration was proposed and adopted to improve the purity level. Finally, the process-level performance of top-performing MOFs (HKST-1, UiO-67) was evaluated on the basis of the experimental isotherms obtained from the literature and compared with the other materials reported in the literature (MIL-100(Fe), UiO-66, and zeolite 13X). We found that the results based on the experimental isotherms are in qualitative agreement with the results based on the simulated isotherms.

Poster Presentation : **MAT.P-437**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Mo-based/CNT/C Composite as Anode Material for the Li-ion Battery

Cu Dang van, Jae Ryeol Jeong, Min Hyung Lee*

Department of Applied Chemistry, Kyung Hee University, Korea

Recently, lithium-ion batteries (LIBs) have been become a candidate for application in electric vehicles. Therefore, many research efforts have been made to exploit LIB material with the high specific capacity and good stability. In this study, the Mo–based/CNT/C composite was synthesized successfully through hydrothermal/annealing processes, and applied for the anode materials in LIBs. Owing the core-shell structure with the super conductivity of the CNT and the homogenous nanoparticle of the Mo–based compounds in amorphous carbon, Mo/CNT/C shows the high specific capacity of 810 mAh g-1 for anode LIBs after 350 cycles at the current density of 100 mA g-1, with a Coulombic efficiency of ~98 %. Our study also reveals that the core-shell structure of Mo/CNT/C with ultrafine nanoparticles of Mo–based compounds contributes to the improvement pseudo-capacitance, resulting in the enhancement of Li ion storage. This research properly opens the new approach in development novel material synthesis for anode LIBs.

Poster Presentation : **MAT.P-438**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Should We use Argon Isotherms to Characterize the Surface Area of Nanoporous Materials?

Seungyun Han, Yongchul Chung[*]

School of Chemical Engineering, Pusan National University, Korea

Surface area is one of the most important physical properties of porous material. Generally, surface areas are determined from a nitrogen adsorption isotherm using the Brunauer–Emmett–Teller (BET) method. However, a recent IUPAC report recommends using an argon adsorption isotherm instead of the nitrogen adsorption isotherm to compute the BET surface area due to the purported "orientational" effect. However, the magnitude of such effect has not been fully characterized in the literature, making it difficult for the community to accept the new standard for porous materials characterization. In this study, we carried out large-scale molecular simulations to investigate the orientational effect of nitrogen and its impact on accurately determining the surface area. The change of the van der Waals interaction between the graphene sheet and gas molecules resulted in a change in the orientation distribution of nitrogen on the monolayer. However, when we compared with nitrogen and argon true monolayer area and geometric area, the differences between Ar true monolayer area and the geometric area did not differ significantly with the differences between N_2 true monolayer area and the geometric area. Finally, we comment on the effect of surface curvature on the orientation of N_2 molecules.

Poster Presentation : **MAT.P-439**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Time-resolved 3D structures of inorganic nanocrystals in oxidative environment revealed by deep-learning assisted one-particle reconstruction

Sungsu Kang, Kim Dongjun, Jungwon Park*

Chemical and Biological Engineering, Seoul National University, Korea

Structural transformation of nanocrystals generally follows nonequilibrium pathways due to their metastable nature. To understand these nonequilibrium pathways, it is essential to understand the exact time-resolved three-dimensional (3D) structures of a nanocrystal undergoing structural transformation in atomic detail. Here, time-resolved 3D structures of dissolving gold and platinum nanocrystals in oxidative environment are investigated via 3D reconstruction of high-resolution liquid cell transmission electron microscopy images combined with neural network-assisted image processing algorithm. The nanocrystal dissolve at different rates, with the fastest dissolution rate just before the complete dissolution. As the nanocrystal dissolves, more fractions of surface atoms are disordered and easier to be detached from the nanocrystal surface. Our methodology will be applied to investigate the time-resolved 3D structures of solvated particles in reactive environment.

Poster Presentation : **MAT.P-440**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

An efficient numerical method for constructing heterojunctions between two crystal lattices using a complex plain

Weon Gyu Lee

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

Important physical properties of two-dimensional (2D) electronic devices are mainly determined by interface geometries in heterojunctions. Here we propose a new numerical method for efficiently constructing heterojunctions between two different crystal lattices having the same in-plane lattice parameter ratio such as a hexagonal graphene-hexagonal MoS_2 heterostructure. The bases of two 2D lattices 1, 2 ((α_{mx}, α_{my}), m=1, 2, α=a, b) can be regarded as the 2D complex vector $l=(z_a\ z_b)$ where ($z_\alpha=\alpha_{mx}+i\alpha_{my}$) in the complex plane. Then, the transformation matrix between two lattices and the complex lattice bases satisfy the eigenvalue problem. We find that a ratio of two lattice matrices $c=|a_{1x}/a_{2x}|$ should be the same as the ratio of norms (h^2+Dk^2) of complex quadratic integers $p=h+k\sqrt{(-D)}$ (h, k are integer, D>0) when two lattices form a commensurate heterostructure. Consequently, using the ratio table, the smallest commensurate heterojunction can be efficiently constructed by finding a quadratic integer without scanning all possible supercells. This is significantly more time-efficient (~O(log n) where n is the maximum value of the transformation matrix elements) than the currently widely used algorithm for construing heterojunctions (~$O(n^4)$).

Poster Presentation : **MAT.P-441**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Limitation of model-based estimations of the hydrogen adsorption capacities of metal-organic frameworks: a molecular simulation study

SungHyun Yun, Yongchul Chung[*]

School of Chemical Engineering, Pusan National University, Korea

There has been a recent report regarding the existence of solid-like H_2 adsorption in nanoporous materials. In this work, we employed grand canonical Monte Carlo (GCMC) simulations on a series of metal-organic frameworks with 1-D and 3-D channels to address the pitfalls of model-based approaches in estimating the hydrogen uptake. The excess hydrogen uptakes of several structures with pore sizes ranging from 5 to 37 angstrom were predicted. The pore volume and the density of adsorbed H_2 were obtained by fitting the Tóth equation to the excess H_2 isotherm data from the simulation, and the results were compared with the data obtained from direct simulation. Sensitivity analyses show that the pore volume and the density of adsorbed H_2, obtained from model-based fitting are not accurate enough to estimate the adsorbed H_2 density and the pore volume of the materials, and especially poor for the materials with 1D channels.

Poster Presentation : **MAT.P-442**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Time-resolved crystallization dynamics of ferritin molecules observed by cryo-EM and liquid-phase TEM

Minyoung Lee, Jungwon Park*

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

Crystallization of biomaterials has been widely used for high-resolution 3D structure reconstruction of protein using X-ray crystallography, and for physiological or pharmaceutical applications in which pure protein samples are crucial. Various mechanisms for nucleation and crystallization of biomaterials have been proposed in previously studies, namely classical nucleation theory, two-step nucleation theory, or desolvation-mediated order-evolution. However, direct observation of nucleation has been difficult due to a lack of techniques that provide the high spatial resolution needed to observe nanoscale nucleates. Herein, we present a single-particle, time-resolved study of equine spleen ferritin crystallization in the presence of CdSO4 using cryo-EM and real-time liquid-phase TEM. Crystallization was observed under different concentrations of ferritin and ionic strengths of the solvent. Using this approach, we elucidate crystallization and nucleation pathways at high resolution and observe dynamics of ferritin crystallization in liquid-phase at a single-molecule level.

Poster Presentation : **MAT.P-443**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Computational investigation of nanoporous materials for highly efficient Xe/Kr separation

Zhao Guobin, Yongchul Chung*

School of Chemical Engineering, Pusan National University, Korea

Xe and Kr gases, are needed in many applications such as illumination, narcotic, and inert probe for nuclear magnetic resonance (NMR). Currently, the pressure swing adsorption (PSA) is considered the most promising separation method because it could greatly reduce the cost and energy consumption of the separation compared to the cryogenic distillation. In this work, based on the CoRE MOFs 2019 and C.U.R.A.T.E.D COFs v9 databases to find high-performing nanoporous materials that can efficiently perform the separation. More than 140 high-performing nanoporous materials identified from molecular simulations were subsequently evaluated based on the ideal adsorption process simulations to evaluate their final performance in the actual process settings.

Poster Presentation : **MAT.P-444**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced photocatalytic degradation of methyl orange on AgBr-SnO_2-carbon nanotube nanocomposites

Seon Jeong Jo, Hyun Chul Choi[1,*]

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

Tin oxide (SnO_2) is an n-type semiconductor that is widely used in a broad range of technical areas as gas sensors, catalysts, battery technology, and transparent electrodes. The use of SnO_2 as a photocatalyst in pollutant degradation and solar energy conversion has been widely investigated because of its high efficiency, photostability, and low toxicity. However, its practical application is restricted by the wide band gap of SnO_2 and the rapid recombination of photogenerated electron–hole pairs. Several recent studies have investigated the utility of combining some semiconductors with different band gaps to form heterojunctions as an effective way to decrease the electron–hole pair recombination rate. Although the enhanced photocatalytic performances are explained by the interfacial interaction, the detailed mechamism are not wll understood. In this study, AgBr–SnO_2 nanocomposites were prepared in the presence of thiolated CNTs. The prepared AgBr–SnO_2–CNT nanocomposites were investigated by means of transmission electron microscopy (TEM), powder X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The photocatalytic activitiesof the AgBr–SnO_2–CNT nanocomposites were evaluated based on the photodegradation of methyl orange (MO). A plausible photocatalytic mechanism is discussed.

Poster Presentation : **MAT.P-445**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Perform Accurate Prediction of Pore Size Distribution Properties in Nanoporous Materials Using Machine Learning

Yu Chen, Seungyun Han, Yongchul Chung*

School of Chemical Engineering, Pusan National University, Korea

Pore size distribution (PSD) is one of the most critical properties to characterize nanoporous materials, especially for gas storage and chemical separation. The current state-of-the-art techniques for obtaining the PSD use an adsorption isotherm as an input to various methods, such as Horvath-Kawazoe, BJH, and Non-Local Density Functional Theory. The adsorption community has widely adopted and routinely used these methods in the literature to characterize new and already synthesized nanoporous materials. However, recent studies in the literature show that these well-established methods can be sensitive to small structural defects. Toward this end, in this work, we developed machine learning (ML) approach using four different algorithms to predict the PSD properties of a class of nanoporous materials such as metal-organic frameworks (MOFs). We compared and discussed the developed ML models with the current state-of-the-art methods.

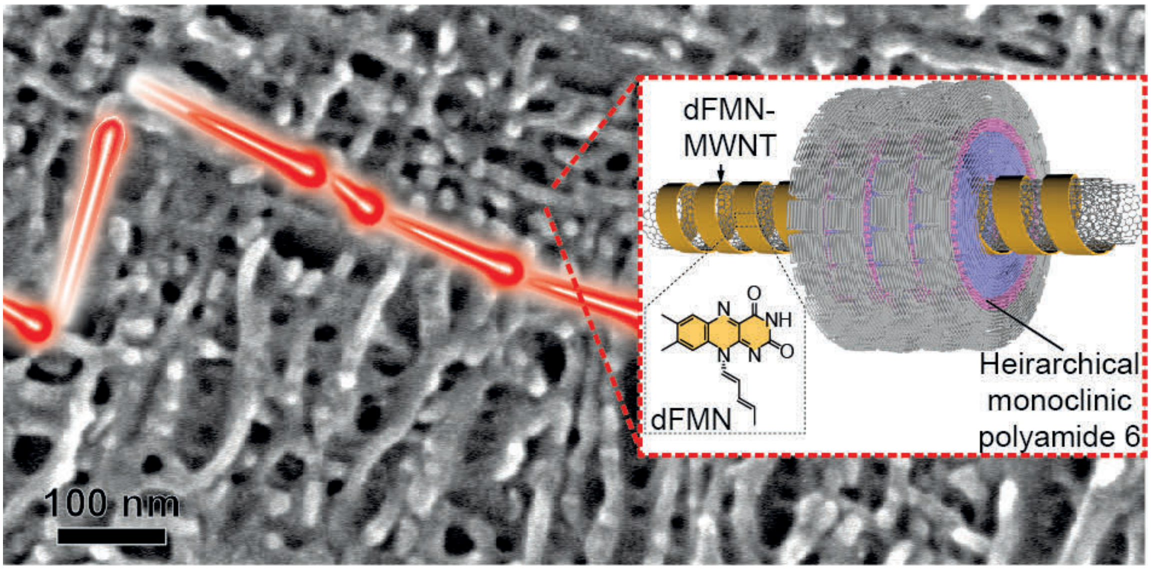
Poster Presentation : **MAT.P-446**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Highly Electrically Conductive Polyamide 6-based Nanocomposite *via* Decomposed Flavin Mediated Hierarchical Monoclinic Multi-walled Carbon Nanotube Structure

Minsuk Park, Sang-Yong Ju[*]

Department of Chemistry, Yonsei University, Korea

Due to the excellent electrical conductivity (σ) of multi-walled carbon nanotube (MWNT), development of nanocomposite with MWNT has been attracting many interests. Especially, polymer-based nanocomposites have the potential to utilize unique properties of MWNT in polymer applications such as sensors, electrodes, and electronics. However, aggregation random distribution of MWNT in a polymer matrix has been problematic.In this presentation, we developed hierarchical monoclinic polyamide 6 (PA)-MWNT nanocomposite with high electrical conductivity. In this approach, MWNT was wrapped by partially decomposed flavin mononucleotide (dFMN) which initially serves as a noncovalent surfactant for individualizing MWNTs. Upon melt extrusion process with PA and MWNT coated by dFMN (dFMN-MWNT), the nanocomposite termed PA-dFMN-MWNT contains monoclinically packed three-dimensional MWNT network embedded in PA matrix. Such well-ordered conductive framework increases σ of the nanocomposite up to 100 S/m, the highest value reported for a polymer-MWNT nanocomposite. X-ray diffraction along with transmission electron microscopy reveal that the presence of dFMN induces the formation of unprecedented α crystalline monoclinic PA on top of dFMN-MWNT and differ in dimensions from that of continuous crystalline phases in PA matrix. In addition, high σ originates minimized defect formation of MWNT by noncovalent functionalization. The nanocomposite exhibit weakened tensile strengths with increasing MWNT content, ascribing mainly to micro voids. The dFMN-MWNT based nanocomposite and their hierarchical structure ordering in this study is expected to be applied easily to make a highly conductive 3D circuits and architectures by being utilized in a 3D printer or the like.


dFMN-
MWNT
N
O
NH
N
N
O
dFMN
Heirarchical
monoclinic
polyamide 6
100 nm

Poster Presentation : **MAT.P-447**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication of a strong graphene oxide composite films through tannic acid based multimodal interactions.

Yoo-Bin Kwon, Young-Kwan Kim*

Department of Chemistry, Dongguk University, Korea

Graphene oxide (GO)-based composite structures are promising candidates for harnessing as structural materials and it is important issue to reinforce their mechanical properties. Tannic acid (TA) is one of the amplest materials in nature with inherent reducing power from galloyl moieties and affinity to the surface of GO sheets through hydrogen bonding. In addition, TA is readily cross-linked by multiple interactions with Fe^{3+} and Polyethyleneimine (PEI) by forming coordination and covalent bonding, respectively. In this study, multi-modal interfacial interactions are explored to form a strong structural material composed of TA functionalized and reduced GO (TA-RGO). TA-RGO was synthesized by simple wet chemistry, and resultant TA-RGO was assembled into artificial nacre-like structure by vacuum-assisted filtration and sequentially cross-liked by Fe^{3+} and PEI to induce formation of a strong interface through multi-modal interactions like π- π interaction, hydrogen, coordination, and covalent bonding. As a result of forming multi-modal interactions, the overall mechanical properties of GO paper were reinforced. We expect that this study presents the efficient and simple strategy for constructing the strong GO-based structural materials.

Poster Presentation : **MAT.P-448**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Eggshell membrane hydrolysate as a eco-friendly reduction agent for synthesis of graphene analogue and its nanocomposite for catalytic application

Junmo Jeon, Young-Kwan Kim[1,*], Ji Hun Park[2,*]

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

Eggshell membrane (ESM) is one of the most attractive and promising food-waste because it has a unique nonwoven fibrous structure mainly composed of collagens with diverse proteoglycans and polysaccharides providing diverse functional groups and chemical potentials. However, the applications of ESM have been restricted owing to low solubility. To address this issue, ESM has been solubilized in aqueous media by enzymatic hydrolysis and thus the resulting ESM hydrolysate (ESMH) can be a promising candidate for chemical synthesis and surface functionalization. Herein, we investigated the application of ESMH for eco-friendly reduction and functionalization of GO. The ESMH-reduced and functionalized GO (ESMH-RGO) exhibited an aqueous dispersibility and applicability as a 2-dimensional support for synthesis of catalytic gold nanoparticles (Au NPs) with a high density. The AuNPs grown ESMH-RGO (AuNPs@ESMH-RGO) presented a high catalytic activity for the conversion of environmental pollutant (4-nitrophenol) to an industrially useful raw material (4-aminophenol). Those results clearly indicate that ESMH has a strong potential in materials chemistry.

Poster Presentation : **MAT.P-449**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Hydrothermal synthesis of TiO_2 nanorods with various aspect ratio and their application to electron transporting material of solar cell

<u>You Jin Park</u>, Wan-In Lee[1,*]

Department of Chemistry and Chemical Engineering, Inha University, Korea
[1]*Department of Chemistry, Inha University, Korea*

TiO_2 nanorods (NRs) of various aspect ratio were selectively synthesized through hydrothermal reaction under basic conditions. Depending on the concentrations of the specific amines added, the obtained titania particles were selectively controlled to 50 nm-sized spherical NP and 70, 85, 100, 120, and 145 nm-length TiO_2 NRs while their widths were kept at 50 nm. The synthesized TiO_2 NRs were in the pure anatase phase and grew to the (101) facet direction during the hydrothermal reaction in basic conditions. Herein, we applied the prepared TiO_2 NRs to the electron transport layer of $FA_xMA_{1-x}Pb(I_xBr_{1-x})_3$ based PSC devices. In overall, TiO_2 NRs provided slightly higher photovoltaic conversion efficiencies (PCEs) than the conventional 50 nm-sized spherical TiO_2 NP. In particular, TiO_2 NR with length of 100 nm (NR 100) provided the highest PCE of 21.00% with J_{SC} of 23.86 mA/cm^2, V_{OC} of 1082 mV, and FF of 0.814. The PCE improvement was mainly due to the increase of FF and V_{OC}.

Poster Presentation : **MAT.P-450**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Composite of Graphite Template and Lithium Iron Phosphate as a Cathode Material for Lithium Ion Battery

KyooSeung Han

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

LiFePO4 has received considerable attention as a cathode material for lithium ion battery because of its low price, environmental benignity, low toxicity, reasonable specific capacity, as well as chemical and electrochemical stabilization. On the other hand, its battery performance is limited by its low electrical conductivity. This is a general characteristic of materials containing polyanions such as phosphate and may lead to extreme polarization during charge and discharge. In addition, its capacity will be markedly reduced if it is not covered in the conducting agent. The electron conductivity of LiFePO4 can be improved by coating it with conducting agents such as graphite or silver nanoparticles. Therefore, carbon-coated LiFePO4 is usually fabricated. Unfortunately, the coated carbon is a mixture of conducting graphite and nonconducting disordered carbon. It is due that the heating temperature during the carbon coating should be under 900°C for the thermal stabilization of LiFePO4. In this way, a composite of graphite template and LiFePO4 is prepared to enhance the electron conductivity of LiFePO4. The preparation procedure of the composite of graphite template and LiFePO4 consists of three steps: (1) coating of graphite on silica balls, (2) elimination of silica to obtain hallow graphite spheres, (3) filling of LiFePO4 in the hallow graphite spheres by Sol-Gel process. The composite of graphite template and LiFePO4//Li cell exhibits the discharge capacity of 161.73 mAh/g (2.0-4.2 V) at a current density of 0.2C, which is 95.2% of the theoretical capacity of LiFePO4. It is also found that both the coulomb efficiency and the energy efficiency of the composite of graphite template and LiFePO4//Li cell are much better than those of the carbon-coated LiFePO4//Li cell.

Poster Presentation : **MAT.P-451**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Porous silicate obtained from industrial waste and its adsorption property in gaseous and aqueous state

Jimin Yeon, Jae-Min Oh[1,*]

Dongguk University, Korea
[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Highly porous silicate materials were successfully prepared by simple acid treatment on industrial waste. Slag which was composed of metal oxides of Si, Ca, Mg, Fe, Mn, and etc. was first ground into powder and the fine powder was separated by 400 mesh (37 microns) sieves. Thus obtained slag powder was treated with either 3 mol/L or 6 mol/L of hydrochloric acid to selectively dissolve metal oxide moieties other than silicon dioxide. According to the nitrogen adsorption-desorption isotherms, the higher concentration of acid produced the larger specific surface area pore volume. According to the pore size distribution analyses, the development of mesopore and micropore was prominent with 3 mol/L and 6 mol/L acid treatment, respectively. The transmission electron microscopic images showed that both silicate materials consisted of small particles of silicon dioxide, of which inter-particle space served as the origin of porosity. The chemical composition of slags and porous silicate was monitored by X-ray photoelectron spectroscopy, suggesting that higher concentration of acid resulted in more dissolution of metal species to result in more pore volume. The adsorption property of thus obtained silicates was studied both in gaseous and aqueous state, showing that both specific surface area and pore size played important role in adsorption performance.

Poster Presentation : **MAT.P-452**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis of solid solutions of $CuCrO_2$ and $CuGaO_2$ and their application to hole transport material of perovskite solar cell

Hyunsue Choo, Woo Seok Suh, Wan-In Lee[1,*]

Chemistry and Chemical Engineering, Inha University, Korea
[1]Department of Chemistry, Inha University, Korea

Copper-based delafossite oxides ($CuMO_2$, M = Cr, Ga, Al, Co, Fe, and others) are expected to be promising inorganic hole transport materials (HTMs) because of their high hole mobility, wide bandgap with high optical transparency, low production cost, and extended chemical stability. They are a kind of 2D-layered structure, consisting of edge-sharing MO_6 octahedra flattened to the direction of c-axis and Cu^{1+} cation located in a trigonal coordination environment. In this work, we synthesized $CuCrO_2$ (CCO), $CuCr_{1-x}Ga_xO_2$ (CGCO, $0 < x < 1$), and $CuGaO_2$ (CGO) by hydrothermal method. Previously, CGO with a high hole mobility is reported to be an efficient HTM for several solar cells, but it is difficult to obtain the pure delafossite phase and to control the particle shape and size. On the other hand, CCO has relatively lower hole mobility, but its particle size can be controlled facilely. Herein, various solid solutions of CCO and CGO were prepared by varying the compositions of Cr to Ga from 1:0 to 0:1. It was found that the CGCO with compositions of 0.4:0.6 exhibited the optimal property with respect to size uniformity and hole mobility. The synthesized CGCO is a hexagonal nanodisc with a size of 5 nm and successfully applied to the hole transporting layer of p-i-n type perovskite solar cells. It was found that the CGCO nanodisc prepared in this work provided PCE of over 14%, which is significantly higher than that of the devices with bare CCO or CGO.

Poster Presentation : **MAT.P-453**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Arc discharge synthesis of graphene with enhanced boron doping levels for electrochemical applications

Chunghun Kim, Myung Jong Kim[1,*]

Department of Nano Science and Technology Convergence, Gachon University Global Campus, Korea
[1]*Department of Chemistry, Gachon University Global Campus, Korea*

Graphene doped with heteroatoms can be applied to various research fields by changing the physicochemical properties of graphene. The most studied dopant so far is nitrogen, but also boron is an element that can supplement and improve the properties of graphene, which are lacking in applied research. Graphene flake synthesis through arc discharge is expected as a method for mass-producing boron-doped graphene flakes, but it has not received much attention due to its low doping rate. In this study, we report the improvement of the doping efficiency of boron-doped graphene synthesized by arc discharge by using a boron precursor and graphene oxide together in an anode carbon filler. As a result of analyzing the doping degree by X-ray photoelectron spectroscopy, the doping level (5.13at%) of the synthesized graphene flakes was significantly higher than that of the boron-doped graphene synthesized by the arc process reported in the previous literature (3at%). Raman spectroscopy demonstrated the movement of the G and 2D bands of the boron-doped graphene flakes, and through this, the structural characteristics of the synthesized graphene flakes can be understood. The boron-doped graphene flakes synthesized by the arc discharge process can be a good electrode material for supercapacitors. CV, EIS, and constant current charge/discharge experiments were performed to observe the electrochemical properties of boron-doped graphene. It is believed that the pseudocapacitance of boron-doped graphene is greater than that of pristine graphene, due to the electron deficiency of substituted boron in graphene. These results suggest that boron-doped graphene flakes required for applied research can be easily provided through an arc discharge process.

Poster Presentation : **MAT.P-454**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Single-crystalline InP tetrapod nanocrystals using surface energy-driven growth

Youngsik Kim, Sohee Jeong[1,*]

Department of Energy Science, Sungkyunkwan university, Korea
[1]*Department of Energy Science, Sungkyunkwan University, Korea*

Colloidal quantum dots (QDs) are semiconductor nanocrystals that their versatile properties can be tuned by the size and surface. Although QDs have been explored for 30 years, an understanding and controlling of the surfaces are still behind, especially, in III-V QD. In this work, we study the controllable colloidal growth in InP QD synthesis using the reaction late intermediates. Through precursor conversion accelerator, almost all monomers are consumed in the nucleation process, thus the nuclei cannot grow into the complete particle, remain as the reaction intermediates. Through TEM analysis, we know that the intermediates have well-defined surfaces as (111) and (110). Based on the understanding of the surface and surface energy, we can control growth direction, and finally, the single-crystalline InP nano-tetrapods having 15 nm arm length are realized. Interestingly, the single-crystalline InP tetrapods have the single-crystalline zinc-blende structure in both center and arm. This result is different from previously reported heterostructure CdSe, CdS tetrapods that have zinc-blende, and wurtzite structures for a center and four arms, respectively. Moreover, the InP tetrapods show novel optical properties.

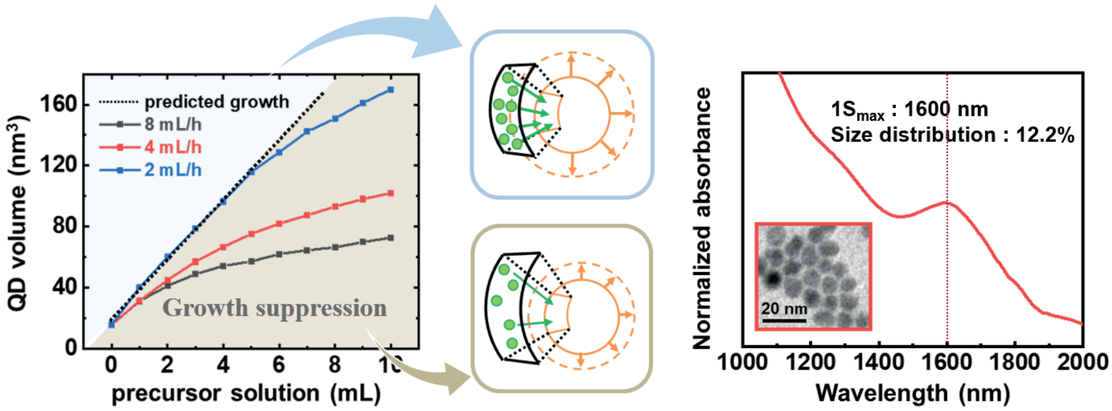
Poster Presentation : **MAT.P-455**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Rational Design Based on Monomer Diffusion Flux Control for Monodisperse and Size-Extended Colloidal InAs Nanocrystals

Seongmin Park, Sohee Jeong*

Department of Energy Science, Sungkyunkwan University, Korea

Colloidal InAs quantum dots (QDs) can exhibit photophysical properties in the short-wavelength infrared (SWIR) region, which can applicate optoelectronics in various infrared fields, such as photodetectors and photovoltaics. Therefore, synthesizing high-quality InAs QDs with optical properties in the SWIR region with narrow size distribution is essential. The hot-injection synthesis strategy using tris(trimethylsilyl)arsine (TMS-As) has been widely reported, but highly reactive arsenic precursor induces rapid depletion of the monomer, which limits the expansion of QD growth. Although a continuous injection system has recently been proposed to synthesize homogeneous and larger-sized InAs QDs, inhomogeneity and growth suppression due to additional nucleation steps or Ostwald ripening events during particle growth limit QD growth expansion. In this study, we propose a growth model of InAs QDs based on the diffusion flux of monomers in a continuous injection system. The experimentally validated model according to various reaction parameters demonstrated that continuous injection of the precursor solution reduced the monomer flux, inhibiting particle growth during synthesis. Consequently, to recover the decreased monomer flux, we synthesize InAs QDs with a size over 9.0 nm (1Smax at 1600 nm) in narrow size distribution (12.2%) by controlling the precursor injection rate and precursor concentration and introducing a diffusion-dynamics-control synthesis method[1].[1]. Kim, T., Park, S. & Jeong, S. Diffusion dynamics controlled colloidal synthesis of highly monodisperse InAs nanocrystals. Nat Commun 12, 3013 (2021).


QD volume (nm^3)
160
120
80
40
0
predicted growth
8 mL/h
4 mL/h
2 mL/h
Growth suppression
0
2
4
6
8
10
precursor solution (mL)
Normalized absorbance
1S$_{max}$: 1600 nm
Size distribution : 12.2%
20 nm
1000
1200
1400
1600
1800
2000
Wavelength (nm)

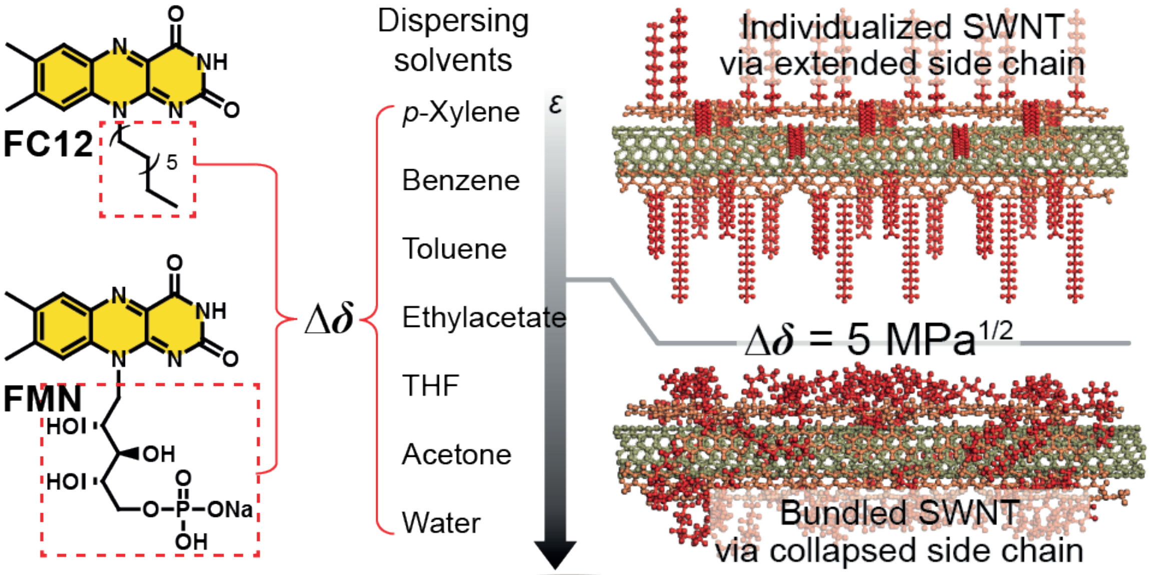
Poster Presentation : **MAT.P-456**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Dispersion of Carbon Nanotubes by Helical Flavin Surfactants: Solubility Parameter induced Stability and Chirality Enrichment, and Solvatochromism in various solvents

Inseung Choi, Minsuk Park[1], Sang-Yong Ju[1,*]

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

Single-walled carbon nanotubes (SWNTs) are a one-dimentional carbon allotrope in the rolled form of a single layer of graphene. SWNTs dispersed in various solvents using various surfactants have wider applications. Despite of the broad application potentials, its solvent-induced properties of dispersion, optical behaviors and their origins are not fully understood because there are no surfactants can disperse SWNTs in various solvents. In this poster, we show solvent-driven properties, chirality selection, and solvatochromism in SWNTs wrapped by two flavin derivatives in various solvents with dielectric constant (ε) ranging from 2.3 to 80.4. Surfactant concentration induced chirality selection is because of binding affinity and stoichiometry relationship of SWNT and surfactant. As solvent ε, dispersions have different distribution of individualized- (iSWNT) and bundled-SWNT (bSWNT), and carbonaceous impurity (CI). Solvents with lower ε lead to iSWNT as a major, but polar higher ε solvents disperse bSWNT or CI as a major. Relative quantum yields of SWNTs have an inverse trend associated with solubility parameter difference ($\Delta\delta$) between solvent and sidechain of surfactant. Dispersion with smaller $\Delta\delta$ leads to iSWNT dispersions, and larger $\Delta\delta$ leads to highly concentrated bSWNT or CI because of mixing enthalpy driven side chain configuration (*i.e.*, extended *vs* collapsed). This result suggests dispersions with smaller $\Delta\delta$ has stable iSWNTs by extended surfactant sidechain configuration, but larger $\Delta\delta$ lead to highly concentrated bSWNT by collapsed sidechain or CI. The results suggest guidelines for design of high-purity and high PL SWNT dispersion for high end applications of SWNT.


FC12
5
FMN
HO
OH
HO
O-P-ONa
OH
Δδ
Dispersing solvents
p-Xylene
Benzene
Toluene
Ethylacetate
THF
Acetone
Water
ε
Individualized SWNT via extended side chain
Δδ = 5 MPa1/2
Bundled SWNT via collapsed side chain

Poster Presentation : **MAT.P-457**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Diameter-Selective Two Phase Extraction of Carbon Nanotubes by an Amphiphilic Poly(2-ethyloxazoline)

Seokhyeon Son, Inseung Choi, Sang-Yong Ju*

Department of Chemistry, Yonsei University, Korea

Single-walled carbon nanotube (SWNT) has physical properties that depend on the direction of a rolling vector (or chiral vector) referred to as a pair of integers (n, m). The separation of SWNT chirality is a prerequisite for high-end optoelectronic applications. Among various SWNT separation methods, aqueous two-phase extraction method based on poly(ethylene oxide)/dextran is advantageous because the process and related cost is affordable. However, this method relies on gradual replacement of two surfactants and, upon replacement of surfactant, provides a relative hydrophilicity against two aqueous phase, leading to chirality separation. However, this method requires multiple extraction steps to discriminate chemical potential differences between SWNT chiralities upon two surfactant replacement.In this poster, we found that an amphiphilic polymeric surfactant not only disperses SWNT in aqueous and organic phases, and, upon mixing two dispersions, but also possesses partitioning of SWNT according to SWNT diameter (dt_2). For this, we utilized poly(2-ethyl oxazoline)-alkylated 2nd generation benzyl ether (POBE) as an universal surfactant for both aqueous and organic phases. Large partitioning of POBE-SWNT is facilitated by a phase transfer catalyst, tetrebutylammonium bromide (TBAB) which showed increased partition constant *K* (SWNT concentration in organic/SWNT concentration in aqeous phase) as increasing TBAB concentration. We have determined chirality-dependent *K* by using absorption spectroscopy. Currently, efforts are being made to create clean phases and interfaces or to increase the number of K for repeated extraction experiments.

Poster Presentation : **MAT.P-458**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Rapid preparation of cobalt based mono- and bi-metallic oxide nanoparticles; highly efficient catalysts for the degradation of organic dyes

Dong-yun Yoon, Hye On Yoon*, Ha-Jin Lee[1,*]

Seoul Center, Korea Basic Science Institute, Korea
[1]*Division of Chemistry and Bio-Environmental Sciences, Seoul Women's University, Korea*

Toxic organic compounds have become major pollutants in water sources, causing serious environment pollution and ecological destruction. In this study, the cobalt based mono- and bi-metallic oxide nanoparticles (NPs) were synthesized by a molten salt method (MSM) within 1 min. The NPs were used as catalysts for rapid degradation of hazardous organic dyes such as methyl orange (MO) and methylene blue (MB) in the presence of peroxymonosulfate (PMS) in aqueous media. In general, cobalt oxide NPs were known to effectively activate PMS to generate sulfate free radicals and degraded toxic organic dyes. Meanwhile, when manganese salts were used as co-precursors with cobalt salts in MSM reaction, cobalt manganese bimetallic oxide nanoparticles (Co/Mn NPs) with various shapes were synthesized depending on their anions. The Co/Mn NPs showed a decomposition efficiency of more than 95% within 2 min in both MB (100 ppm) and MO (100 ppm) solutions. Our study presents a facile pathway synthesizing Co/Mn nanoparticles with efficient catalytic degradation activity of organic dyes.Acknowledgements: This study was supported by the National Research Foundation of Korea (NRF) grant (Project No. NRF-2019R1A2C2007092).

Poster Presentation : **MAT.P-459**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Detection of fast and sensitive target molecules by aptamer-based TFT bio-sensor that can be reused through real-time detection.

Yong Wan Kim, Young-Geun Ha[1,*]

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

The disadvantage of conventional disease diagnosis is that it takes a lot of time and costs to go to the hospital for a checkup and cannot be diagnosed in real time. This study has the advantage of reducing the time and cost of diagnosing existing diseases by using aptamer-based TFT Bio-sensor, which is reusable and real-time detectable. 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. Aptamer is smaller than antibodies, stable at room temperature, and stable at pH changes, allowing for reusable sensors. For reuse, the pH of the rinse solution is adjusted to make the target molecules fall, and for real-time detection, PDMS cells are made to allow real-time detection by making the target molecules flow to the channel. When a solution containing a target molecule is spilled, it can be detected and detected sensitively. When a separation solution is spilled, the target molecule is separated from the aptamer, so an aptamer-based TFT Bio-sensor that can be reused and detected in real time is fabricated.

Poster Presentation : **MAT.P-460**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Preparation of robust, self-healing superhydrophobic fabrics through simple solution process at room temperature

Su Yeon Jeong, Young-Geun Ha[1,*]

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

The lotus leaf is one of the most studied superhydrophobic surfaces found in nature, which has a water contact angle(WCA) above 150° and an sliding angle below 5°. Over the past decade, superhydrophobic surfaces found in nature has led to the development of a number of artificial superhydrophobic coatings and these are being in real life. In this experiment, a superhydrophobic fabric was produced through a solution process at room temperature. We applied a layer of ZrOx solution onto the fabric at room temperature. And we obtained a rough surface through self-assembled monolayer(SAM) using octadecylphosphonic acid (ODPA) which has a long alkyl group and contributes to low surface energy. The fabric produced was modified to a surface result in a water contact angle greater than 150° and an sliding angle smaller than 10°. The coated surface still retained the superhydrophobicity after physical and chemical damage and has self-healing ability. The presented method can be applied not only to various fabrics, but also to various substrates such as silicon and glass, and through excellent superhydrophobicity and a simple manufacturing method, a surface that can be applied to wide range of practical applications.

Poster Presentation : **MAT.P-461**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Cancer Theragnostics by Rhodamine B-loaded Mesoporous Silica-coated Gold Nanorods

Yu Ra Lim, Hyowon Han, Ara Joe, Eue-Soon Jang*

Department of Applied Chemistry, Kumoh National Institute of Technology, Korea

We synthesized cetyltrimethylammonium bromide (CTAB)-templated mesoporous silica coated gold nanorod (CGNR@*m*SiO$_2$) to enhance drug-loading capacity. However, we found that the CGNR@*m*SiO$_2$ nanocomposites have a high cytotoxicity due to residual CTAB surfactant even after the washing process. Calcination is common procedure to eliminate the CTAB from the mesoporous silica frameworks. However, we confirmed the dissolution of the core GNR at a calcination temperature of 300-600 ℃, which causes a blue-shift in the longitudinal surface plasmon resonance (LSPR) mode of the core GNR from the NIR to visible wavelength. On the other hand, we found that substitution method *via* amine-functionalized fluorescence dyes such as methylene blue (MB) and rhodamine B (RB) is excellent procedure not only to reduce the cytotoxicity of the CGNR@*m*SiO$_2$ but also to explore new cancer theragnostic agents. Among them, the RB molecules were more effective in replacing the CTAB in the CGNR@*m*SiO$_2$ than the effect exhibited by MB molecules because its positive ζ potential induced a strong binding affinity to the core GNR. In particular, the RB-CGNR@SiO$_2$ showed superior cancer therapeutic effect by generation of abundant reactive oxygen species (ROS) under near-infrared (NIR) excitation light. Therefore, it is indicating that the RB-CGNR@SiO$_2$ nanocomposites promise the new cancer theragnostic agent with biocompatibility.

This research was supported by the research fund of the Korean Ministry of Education, Science & Technology (2016R1D1A3B0201175615) and the Grand Information Technology Research Center Program (1711120024) through the Institute of Information & Communications Technology Planning & Evaluation (IITP) funded by the Ministry of Science and ICT (MICT), Korea.

Poster Presentation : **MAT.P-462**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis of Zn-doped InAs colloidal quantum dots with p-type polarity

Hyoin Kim, Sohee Jeong*

Department of Energy Science, Sungkyunkwan University, Korea

Colloidal quantum dots (CQDs) have wide tunability on optical, and electrical properties due to size dependent quantum confinement effect. This leads CQDs as promising materials for optoelectronic devices such as solar cell, light emitting diode, photodetector. However, doping in CQDs is more challenging compared to bulk semiconductor, in which carrier type can be easily controlled by impurity doping. As-synthesized CQDs with cation-rich surfaces commonly show n-type transport behavior. There have been attempts to change majority carrier by impurities doping, stoichiometry control, and ligand exchange, but p-type CQDs have been rarely reported. Also, most of them are lead based CQDs, which have to be changed by alternatives with less toxicity. Here, we synthesized Zn-doped InAs CQDs. In this system, zinc successfully incorporated during InAs CQDs synthesis and p-type transport behavior was confirmed by field effect transistor measurement.

Poster Presentation : **MAT.P-463**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Tuning Energy Level of Indium Phosphide Films Through the Ligand Modification

Eunhye Cho, Mahnmin Choi, Sohee Jeong*

Department of Energy Science, Sungkyunkwan University, Korea

Colloidal quantum dots (CQDs) are promising materials due to their tunable properties by changing their size and surface environment. Given their tunable properties, they can be applied to various devices such as display, photovoltaics, bio-imaging. In the various device, it is important to control the energy level which can be shifted by the ligand-induced dipole on the surface of the nanocrystal. 3-5 group QDs, although promising alternative materials due to low toxicity, are lagging the study of tuning the energy level. Moreover, the synthesis of the 3-5 group cannot avoid surface oxidation which complicates interpreting the factor of energy level shift. In this work, we analyze the energy level of Indium Phosphide (InP) controlling the ligand-induced dipole. Moreover, we can exclude surface oxidation through acid-free synthesis. The ambient Photoemission Spectroscopy measurement allows us to clearly analyze the valence band edge of InP film and resolve the charge-up problem. In addition, we confirm that the surface of InP QDs was not oxidated using X-ray Photoemission Spectroscopy.

Poster Presentation : **MAT.P-464**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Aptamer activated-multiwall carbon nanotube network on filter paper to detect beta-amyloid for Alzheimer's disease diagnosis.

Jeong Eun Kim, JiHyeon Mun, Sumin Kim, Jiyeong Park, Don Kim*

Department of Chemistry, Pukyong National University, Korea

The most believed biomarkers to monitor Alzheimer's diseases (AD) are beta-amyloid (β-A) peptides. A high β-A level makes aggregation in the brain and causes dementia. The detection of β-A requires sensitive and expensive sophisticated instruments and is not applied at point-of-care (POC). We present an inexpensive, easy, fast method to assay β-A with aptamer-activated multiwall carbon nanotubes (MWCNTs). The activated MWCNTs were deposited on filter paper to use as β-A immunosensor sensors. In the preliminary test, the sensor could assay the β-A within 90 min, with and analytical sensitivity of 0.00525 (ng/ml)-1 with a limit of detection of 3.0 ng/mL in the range of 0 – 80 ng/mL β-A. This method is much faster than enzyme-linked immunosorbent assay (ELISA, 6 h), but it still needs improvement and optimization of its performance to apply for POC.

Poster Presentation : **MAT.P-465**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

EFFICIENT IR PHOTOVOLTAICS USING INDIUM ARSENIDE COLLOIDAL QUANTUM DOT AS ELECTRON TRANSPORT LAYER

Daekwon Shin, Sohee Jeong*

Department of Energy Science, Sungkyunkwan University, Korea

Most materials in current photovoltaics (PVs) fail to harvest photons in the IR range as they have bandgaps larger than 1.1 eV. On the contrary, colloidal quantum dots (CQDs) allow us to harvest IR range by tuning their bandgap (below 1.1 eV) by controlling their size. Hence, CQD PVs provide an opportunity to overcome Shockley-Queisser single junction efficiency limit when used as a bottom cell in a tandem structure. Conventionally, best performing CQD PVs have adopted PbS CQD as the active layer and n-type ZnO as an electron-transport layer (ETL). However, ZnO is not suitable for IR PVs as they require UV activation to function effectively. Thus, we suggest using InAs CQD film as ETL for IR PVs. Herein, we synthesized the InAs CQD using the continuous injection method and reconstructed the surface of InAs CQDs via two-step surface modification: First, peeling of native ligands on the surface, then passivating with short ligands. The above-mentioned InAs CQD film was analyzed by x-ray photoelectron spectroscopy (XPS) and field-effect transistor (FET) current-voltage (I-V) curves. We confirmed that the surface of InAs CQD was successfully reconstructed, and the InAs CQD film has an n-type doping feature through XPS and FET I-V curves respectively. Lastly, we fabricated IR PVs using InAs CQD in place of ZnO and evaluated the IR performance as the tandem bottom cell. As a result, the ZnO device showed S-shaped I-V curve whereas the InAs CQD device showed rectifying I-V curve indicating efficient electron transport. Plus, the device with InAs CQD ETL showed reduced hysteresis in comparison to the one with ZnO ETL. We believe that this study proposed a promising alternative for optoelectronics aiming to utilize the IR band.

Poster Presentation : **MAT.P-466**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Evaluation of size effect on layered double hydroxide for phosphate removal to wastewater

Tae-Hyun Kim

Department of Environmental Engineering, Seoul National University of Science & Technology, Korea

Phosphorous (P) in the form of phosphate is an essential nutrient for eco-system and most of the P is obtained by mining from phosphate rocks which is a limited resource that may be depleted within decades. The wastewater from wastewater treatment plants (WWTPs) could be alternative phosphate source due to the high concentration of phosphate (5-20 mgP/L). To recover phosphate from phosphate rich water-system, layered double hydroxide (LDH) have been widely studied due to their favorable properties such as biocompatibility, high affinity and high adsorption capacity for orthophosphate. Three different MgAl layered double hydroxide intercalated chloride anion and lateral sizes in the range 70 to 300 nm were prepared by conventional coprecipitation method followed by hydrothermal treatment at 100℃ (12 h), 150℃ (24 h) and 120℃ (96 h) for LDH-S, LDH-M and LDH-L, respectively. All MgAl-LDH shows typical hydrotalcite-like structure according to Powder X-ray diffraction. The particle size, morphology and surface charge of the MgAl-LDH were verified by electron microscopic analysis, elemental analysis, zeta-potentiometer and dynamic light scattering. Moreover, multi-nuclear solid state NMR was used to understand the atomic level of structure of MgAl-LDH. Then, the phosphate adsorption capacity and recyclability of three different lateral size of MgAl- LDH were evaluated as a function of exposure time, phosphate concentration and using simulated phosphate solution and wastewater (reject water). The obtained solid products were analyzed by analytical protocol above as well analysis of the supernatant to probe the LDH stability during phosphate exposure.

Poster Presentation : **MAT.P-467**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Fabrication of biosensor based on amorphous oxide semiconductor IGZO

Jihyeon Kim, Young-Geun Ha[1,*]

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

Field effect transistors (FETs) are being used in various ways in the field of biosensors. FET is a transistor through which carriers flow by an electric field when a voltage is applied to the gate electrode. Metal oxide is mainly used as a semiconductor material for FETs. It is well known that metal oxides are unstable to bias stress. Indium oxide, which is generally used, is particularly unstable, and IGZO semiconductor is applied to compensate for this. The sensor was fabricated by fabricating IGZO under the conditions with the least effect of positive bias stress (PBS), and the rate of change of current according to the increase in Tau381 concentration at positively applied voltage was analyzed over time. The Tau381 detection change rate over time in this study shows the potential for future development as a real-time sensor. In addition, the sol-gel process of the semiconductor film and the surface treatment of the sensing region are performed through a solution process, which has the advantage of being able to fabricate the sensor in a simple and low-cost method.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **MAT.P-468**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Easy access to arylboron dichloride from arylboronic acid with tetrachlorosilane

Soyeon Cheon, Young S. Park*

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

Heteroatom doping is a general strategy for the purpose of modulating electronic property of organic semiconducting materials. In particular, the isoelectronic substitutions of carbon and carbon (CC) bonds with boron and nitrogen (BN) bonds in the molecule enable its electronic property to be fine-tuned without significant structural changes. To construct BN bonds, the halogenated boron reagents such as arylboron dichloride reacting with amine groups are key components in the reaction. However, commercially available arylboron dihalide lacks its diversity compared with the corresponding arylboronic acid. Moreover, there have been only a limited number of methods for preparing arylboron dichloride so far. Herein, we report a convenient synthetic protocol for the formation of a variety of arylboron dichlorides from arylboronic acids with tetrachlorosilane. By using this method, we demonstrate the straightforward synthesis of BN-ixene, where the location of B and N atom is precisely controlled. Our simple and convenient method can pave the way for developing a wide range of BN-containing molecules.

Poster Presentation : **MAT.P-469**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Effects of Heteroatom-Doping in Tetraphenylnaphthalenes

<u>Jupil Park</u>, Young S. Park*

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

In the past few decades, many studies on semiconducting electronic organic materials to replace traditional inorganic materials have been conducted. In order to improve the performance of organic electronic devices, the atomistic bandgap engineering strategy for controlling the optical and electronic properties of constituent molecules has been proposed. The atomistic bandgap engineering strategy modulates the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels by replacing certain atoms in the molecular structure with atoms from other elements. Herein, we report the synthesis and characterization of heteroatom-doped 1,2,3,4-tetraphenylnaphthalene (TPN) derivatives in which the carbon–carbon (CC) bond is replaced by either a boron–nitrogen (BN) bond or a phosphorus–nitrogen (PN) bond. In this study, we developed a new synthetic strategy for the formation of a BN or PN bond and the simultaneous introduction of a halogen group into the naphthalene core. Subsequently, we performed the palladium-catalyzed cross-coupling reactions to attach the phenyl groups. This approach developed herein would enable modular syntheses by varying diverse aryl substituents on 2,1-borazaronaphthalene and 1,2-azaphosphine cores via sequential cross-coupling reactions.

Poster Presentation : **MAT.P-470**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Efforts toward synthesis of BN-doped hexa-*peri*-hexabenzocoronene

Kidal Kwon, Young S. Park[*]

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

The introduction of heteroatom is a powerful tool to control the electronic properties of carbon-based molecules such as polycyclic aromatic hydrocarbons (PAHs). As one interesting example of PAHs, hexa-*peri*-hexabenzocoronene (HBC) has received much attention as electronic materials due to its large π-conjugation. There have been reported only two examples of HBCs containing borazine (B_3N_3) core, but has no precedent for HBC with one boron and nitrogen (BN) unit in the core. Herein, we report the synthetic progress toward HBC with 1,2-azaborine core. In this study, we provide many attempts for the introduction of a BN bond and the subsequent carbon and carbon (CC) bond formation.

Poster Presentation : **MAT.P-471**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

MXsoprtion of mercury: Exceptional reductive behavior of titanium carbonitride MXene

Asif Shahzad[*], **Jae-Min Oh**[*]

Department of Energy and Materials Engineering, Dongguk University, Korea

Two-dimensional transition metal carbides and nitrides (MXenes) have drawn attention for application in the environmental remediation realm. In this study, we reported the simultaneous reductive-adsorption behavior of titanium carbonitride (Ti3CNTx) for toxic metal ion mercury (Hg2+) in the aqueous phase. Two-dimensional Ti3CNTx and Ti3C2Tx MXene nanosheets were synthesized by exfoliation of Ti3AlCN and Ti3AlC2 MAX phases. The fabricated MXene nanosheets were used to investigate their Hg2+ removal, Hg2+ intercalation, and surface interaction mechanism efficiency. Both MXene family members were found to adsorb and reduce a larger amount of Hg2+. Analytical techniques such as X-ray powder diffraction, field emission transmission electron microscopy, zeta-potential analyses, and X-ray photoelectron spectroscopy were used to investigate the material characteristics and structural changes after mercuric-ion uptake. The quantitative investigation confirmed the interaction of bimetal and hydroxyl groups with Hg2+ using electrostatic interactions and adsorption-coupled reduction. In addition, both MXenes exhibited extraordinary mercury-removal capabilities in terms of fast kinetics with an excellent distribution coefficient up to 1.36 × 10+9. Based on batch adsorption results, Ti3C2Tx and Ti3CNTx exhibited the removal density of 5473.13 and 4606.04 mg/g, respectively, for Hg2+, which are higher values than those of previous mercury adsorbents.

Poster Presentation : **MAT.P-472**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Toward the synthesis of isomeric ixene derivatives

Seongrok Shin, Young S. Park[*]

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

Polycyclic aromatic hydrocarbons (PAHs) are in a category of π-conjugated organic compounds, which are composed of fused benzene rings. PAHs are commonly electron-rich, so that can be utilized as semiconducting organic electronic materials. Extension of π-conjugation can be a method for tunning optoelectronic properties of molecules, usually by lowering bandgap energy. Herein, we prepare the isomeric ixene derivatives (i.e., dibenzo[*b*,*q*]ixene and dibenzo[*c*,*r*]ixene) by controlling the connectivity of naphthalene rings during the synthesis. In this study, we adopted ixene molecule as a core motif and installed additional aromatic rings to its specific position by selective C–H arylation reactions. The optoelectronic properties of molecules associated with the structural variations will be discussed.

Poster Presentation : **MAT.P-473**

Material Chemistry

Exhibition Hall 1 THU 11:00~12:30

Gap Hydrothermal Synthesis for Conformal Deposition of Nanostructured Hematite Thin Films for Efficient Photoelectrochemical Water Oxidation

Heejung Kong

Department of Physics, Kyungpook National University, Korea

It is hard to achieve the high performance of hematite (α-Fe_2O_3) in a solar water splitting cell because of its very short carrier lifetime and considerable hole trapping at surface states. In this report, we introduce a novel hydrothermal synthesis method called gap hydrothermal synthesis (GAP-HS) for conformal deposition of the nanostructured hematite thin films on the fluorine-doped tin oxide (FTO) substrates. The hematite thin films synthesized via GAP-HS showed an extraordinary shape with an enlarged surface area and thin thickness, thereby reducing the carrier recombination rates both in bulk and at the surface. This nanostructure produced a high photocurrent of more than 1.2 mA cm^{-2} by only annealing at 550 °C. To the best of our knowledge, this is the highest photocurrent generated by the pristine hematite photoanode obtained by hydrothermal synthesis. Moreover, GAP-HS exhibited an interesting phenomenon associated with the growth of the nanostructure that reflects the grain morphology of the substrate. It is expected that GAP-HS can be applied to synthesize the nanostructured thin films of other materials.

Poster Presentation : **MAT.P-474**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Dehydrated Hydrotalcite–Niclosamide Nanohybrid as Drug Delivery Strategy towards SARS-CoV-2 Viral Infections

Sieun Park, Goeun Choi[1,*], Huiyan Piao[2], Sanoj Rejinold Nirichan[2], Seungjin Yu, Geunwoo Jin[3], Jin-Ho Choy[4,*]

a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. Department of Chemistry, Dankook University, Korea

[1]*a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. Department of Nanobiomedical Science, c. College of Science and Technology, Dankook University, Korea*

[2]*Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), Dankook University, Korea*

[3]*Research Center, CnPharm, Korea*

[4]*a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. Department of Pre-medical Course, College of Medicine, Dankook University, Korea*

COVID-19 has been affecting millions of individuals worldwide and, thus far, there is no accurate therapeutic strategy. This critical situation necessitates novel formulations for already existing, FDA approved, but poorly absorbable drug candidates, such as niclosamide (NIC), which is of great relevance. In this context, we have rationally designed NIC-loaded hydrotalcite composite nanohybrids, which were further coated with Tween 60 or hydroxypropyl methyl cellulose (HPMC), and characterized them in vitro. The optimized nanohybrids showed particle sizes

Poster Presentation : **MAT.P-475**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Direct-labeling Synthesis of TiO_2@MnO_2 Nanoparticles with Zirconium-89 for Cancer Cell Treatment.

Jeong hoon Park[*], **Pyeong Seok Choi**

Accelerator Radioisotope Develolpment, Korea Atomic Energy Research Institute, Korea

Nanoparticles having the properties to target cancer cells by enhancement of the permeability and retention (EPR) effect have been applied to study in vivo tumor diagnosis and treatment. The utilization of zirconium-89 (^{89}Zr) with the nanoparticles can assist track their pharmacokinetics due to relatively long half-life. Here, in this study, we synthesized ^{89}Zr ions labeled inside of titanium oxide nanoparticles through simple one-pot direct-labeling method. Zr-89 is combined with the nanoparticles during their crystal growth occurred. The round-shaped titanium oxide nanoparticles was obtained after 24 h of hydrothermal reaction with ^{89}Zr-chloride and citric acid, then MnO_2 shell was introduced on the surface of ^{89}Zr-TiO_2. As a results, the higher ^{89}Zr-labeling yield in the TiO_2@MnO_2 nanoparticles (≥95%) was obtained, and its labeling stability was significantly high (≥99%) in physiological environment for the span of a week in comparison with post-labeling on the particles with ^{89}Zr. For its biological applications, the in-vitro cell uptake showed that it rapidly internalized in CT-26 cancer cells and increased over the incubation time. We also evaluated cell viability of the CT-26 cancer cells to confirm its capability of the cancer cell treatment. ^{89}Zr-TiO_2@MnO_2 nanoparticles showed significant toxicity for the CT-26 cancer cells in 24 h. In conclusion, Zr-89 labeled TiO_2@MnO_2 nanoparticles could be effective to treat cancer cells because of their high stability in biological environments and specific cancer cell toxicity. The radioactive nanomaterials have a possible applicability for cancer therapy.

Poster Presentation : **MAT.P-476**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Improving quantum dot solar cell performance by reducing open-circuit voltage deficit of PbS QD.

Chaeyeon Lim, Sohee Jeong[1,*]

department of energy science, Sungkyunkwan University, Korea
[1]*Department of Energy Science, Sungkyunkwan University, Korea*

Colloidal quantum dot (CQD) solar cell is an emerging next generation solar cell based on its band gap tunability and solution processability. To develop strategies for continued improvement in CQD solar cell, a better understanding of the factors that degrade their performance is essential. In particular, it is important to address the issue of large open-circuit voltage (VOC) deficit which is a major problem in reaching higher efficiencies.Here, we fabricated a PbS CQD solar cell with an ITO/ZnO/PbS-I/PbS-EDT structure and studied the different material properties according to the ZnO film manufacturing method. In particular, we analyzed origin of the high VOC deficit through energy bands that change with ZnO film annealing temperature and time.Through this process, we improved the large VOC deficit and optimized the PbS CQD solar cells condition. As a result, we achieved the efficiencies of PbS QD solar cells with significantly improved performance compared to the non-optimized one.

Poster Presentation : **MAT.P-477**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Bio-material based adsorbent for heavy metal ion trapping

<u>Jungho Chae</u>, Jeong Hoon Park*

Accelerator Radioisotope Development, Korea Atomic Energy Research Institute, Korea

In this study, a natural product-based natural adsorbent was synthesized to remove major heavy metals contained in industrial wastewater discharged in Korea. Heavy metals generated through industrial wastewater include Cr, Ni, Cu, Zn, Cd, and Pb in common, and since they are not naturally biodegradable or purified, they accumulate in living organisms and adversely affect the human body. The natural product-based adsorbent synthesized PC beads (Pectin + Chitosan beads) through cross-linking of pectin and chitosan. Pectin is made of galacturonic acid as a monomer and is rich in carboxyl and hydroxyl groups, it has a strong affinity for many metal ions, so it is spotlighted as a promising natural adsorbent. Chitosan is a derivative of chitin, has a structure similar to that of cellulose, and contains amine and carboxyl groups that can effectively bind heavy metals, so it is widely used as an adsorbent. To compensate for the low mechanical strength of pectin, different ratios of pectin and chitosan (10:0, 8:2, 6:4, 4;6, 2:8, 0:10) were synthesized by adding chitosan. The physicochemical properties of the synthesized PC beads were evaluated through FTIR, SEM, and EDS. As for structural properties, the average diameter was about 2.5 mm, and a mesoporous structure was formed as the content of pectin was increased. In order to compare the heavy metal adsorption capacity according to the actual environment of wastewater, the distribution coefficient (K_d) was evaluated under different reaction conditions (time, pH), and the possibility of its use as an adsorbent for industrial wastewater was confirmed.

Poster Presentation : **MAT.P-478**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Layered Double Hydroxide-Nicotinic Acid Nanohybrids for Controlled Drug Delivery System

Seungjin Yu, **Huiyan Piao[1]**, **Goeun Choi[2,*]**, **Jin-Ho Choy[3,*]**

a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. Department of Chemistry, Dankook University, Korea
[1]*Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), Dankook University, Korea*
[2]*a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. Department of Nanobiomedical Science, c. College of Science and Technology, Dankook University, Korea*
[3]*a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. Department of Pre-medical Course, College of Medicine, Dankook University, Korea*

Nicotinic acid (NA), known as Vitamin B3 has a variety of pharmaceutical and dermatological functions such as effective skin whitening, and anti-inflammatory properties. However, high dosage administration of NA could lead to dermatological side effects such as erythema and itching. Therefore it is necessary to develop the NA delivery carrier with controlled release property. Recently, we successfully developed delivery system with slow release property incorporating NA into interlayers of layered double hydroxide (LDH) via co-precipitation method. According to the X-ray diffraction analysis, the basal spacing of NA-LDH nanohybrid was determined to be 1.55 nm indicating that the NA molecules were successfully intercalated into the interlayer space of LDH. The release profile in the gastrointestinal solution confirmed that NA was controlled release in the NA-LDH-Polymer nanohybrids. And therefore, we suggest that NA-LDH-Polymer nanohybrids may have a potential application as the controlled drug release system.

Poster Presentation : **MAT.P-479**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Niclosamide loaded in mesoporous silica and aluminosilicate; potential drug delivery systems for COVID-19

Huiyan Piao, Sanoj Rejinold Nirichan, Goeun Choi[1], Geunwoo Jin[2], Jin-Ho Choy[3,*]

Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), Dankook University, Korea
[1]*a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. College of Science and Technology, Dankook University, Korea*
[2]*Research Center, CnPharm, Korea*
[3]*a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. Department of Pre-medical Course, College of Medicine, Dankook University, Korea*

COVID-19 is rapidly spreading under the fourth wave, for which there has been no specific medication found yet. Therefore, it is necessary to find a solution for this ongoing pandemic with the aid of advanced pharmaceutics. What is proposed here as a solution is the repurposing of FDA-approved drug such as niclosamide (NIC) having multiple pathways to inactivate the SARS-CoV-2, the specific virion, that induces COVID-19. However, NIC is hardly soluble in an aqueous solution, thereby poor bioavailability resulting in low drug efficacy. To overcome such a disadvantage, we propose here an oral formulation based on Tween 60 coated drug delivery system comprised of three different mesoporous silica and aluminosilicates like MCM-41, SBA-15, and geopolymer hybridized with NIC molecules. According to the in-vitro release studies under a gastro/intestinal solution, the cumulative NIC release out of NIC-silica nanohybrids was found to be greatly enhanced to ~97% compared to the solubility of intact NIC (~40%) under the same condition. We also confirmed the therapeutically relevant bioavailability for NIC by performing pharmacokinetic (PK) studies in rats with NIC-silica oral formulations. In addition, we discussed in detail how the PK parameters could be altered not only by the engineered porous structure and property, but also by the dipolar interaction between NIC-NIC and the van der Waals one between pore wall-NIC in the intra-pores of silica nanoparticles, as well as the ion-dipolar interaction between intrapore cation-NIC of aluminosilicate one.

Poster Presentation : **MAT.P-480**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Injectable Niclosamide Hybrid Nanoparticles Towards SARS-CoV-2 Therapy

Sanoj Rejinold Nirichan, Huiyan Piao, Geunwoo Jin[1], Goeun Choi[2,*], Jin-Ho Choy[3,*]

Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), Dankook University, Korea
[1]*Research Center, CnPharm, Korea*
[2]*a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. College of Science and Technology, Dankook University, Korea*
[3]*a. Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), b. Department of Pre-medical Course, College of Medicine, Dankook University, Korea*

COVID-19 is a rapidly evolving emergency, which necessitates the scientific community to come up with an effective remedy for fast recovery of the millions affected around the globe. Even though FDA initially approved Remdesivir as an injectable drug for COVID-19, later on it was failed to retain the claims, thereby WHO rejected its further use. Hence, it is of utmost importance to develop effective and affordable injectable drug medications to treat the ongoing pandemic. The present work reports a formulation based on poly ethylene glycol (PEG), which is coated on bovine serum albumin (BSA) stabilized Niclosamide (NIC) nanoparticles (NPs) (~ BSA-NIC-PEG NPs) as an injectable formulation. The serum albumin mediated strategy is proposed as an effective strategy to enable selectively target SARS-CoV-2 virus that causes COVID-19. The as made readily water dispersible formulation (size

Poster Presentation : **MAT.P-481**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Photoelectron Yield Spectroscopic Studies on Band Edge Position of Insulating QD Films

Mahnmin Choi, Sohee Jeong[1,*]

Department of energy science, Sungkyunkwan University, Korea
[1]*Department of Energy Science, Sungkyunkwan University, Korea*

Tunable band edge position of quantum dots (QDs) is essential character to improve the performance of various QD-based applications. Yet, the investigation of the band edge positions in insulating QD films have been insufficient. Here we study band edge position of insulating QD films using photoelectron yield spectroscopy. While the photoelectron spectroscopic measurement of insulating QD films undergo inevitable charge-up problem, photoelectron yield spectroscopy accurately measured band edge position of insulating QD films. In addition, we find that photoelectron yield spectroscopy can measure the band edge positions irrespective of the kids of substrates, from metallic to large bandgap semiconductor. We further evaluate the shift of band edge position linearly through controlling dipole layer on QD surface. This study provides the understanding on the band edge position of insulating QD which is critically suggested future optimization of band structure for QD-based applications.

Poster Presentation : **MAT.P-482**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Study on InAs amorphous cluster and magic-sized cluster: characteristics as a precursor

Jibin Shin, Youngsik Kim[1], Mahnmin Choi[2], Sohee Jeong[*]

Department of Energy Science, Sungkyunkwan University, Korea
[1]*Department of Energy Science, Sungkyunkwan university, Korea*
[2]*Department of energy science, Sungkyunkwan University, Korea*

Nanocrystal formation typically does not follow classical nucleation and growth model well due to their complex reaction pathway originated from the drastic surface changes (e.g., facets, edges, and vertexes) in particle formation. In the complex reaction pathway, local minima energy states of the particle inevitably exist, and thus various intermediate particles called nanoclusters have been shown. For some quantum dots (QDs), including InP, the studies of clusters have been actively conducted into the structure, surface chemistry, and the role as a building block or a precursor. However, there has not been much study on InAs cluster despite their potential uses. Only a few studies show that the InAs magic-sized cluster (MSC) has a distinct absorption peak at 420 and 460 nm but there are no studies about the structural and surface characteristics of InAs cluster. In this study, we analyze and compare InAs MSC synthesized with indium acetate and InAs amorphous clusters previously used as a precursor in our lab. Thermal stabilities of the clusters are evaluated by measuring the activation energy of the conversion from cluster to QD. As a result, we suggest the characteristics of both clusters as a precursor of InAs QD synthesis.

Poster Presentation : **MAT.P-483**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Controlling molecular arrangement of deoxycholic acid utilizing 2-dimensional layered double hydroxide

Hyeonjin Park, Jae-Min Oh[1,*]

Department of energy and materials engineering, Dongguk University, Korea
[1]*Department of Energy and Materials Engineering, Dongguk University, Korea*

Deoxycholic acid (DA), a metabolic byproduct in living system is known to have various biological functionality; however, its sensitive molecular aggregation hindered its practical applications. In this study, we controlled the molecular aggregation utilizing layered double hydroxide (LDH) as 2-dimensional partition. We hybridized DA and LDH through three different reactions, coprecipitation, ion exchange, and reconstruction, which are representative methods to get organic-LDH hybrids. According to X-ray diffraction pattern, it was shown that only reconstruction was effective in achieving molecular arrangement of DA in LDH through partial intercalation. Elemental analysis data also showed that coprecipitation and ion exchange routes produced DA-LDH mixtures with very high organic content, while reconstruction showed reasonable ratio between organic and LDH part to be a hybrid. Both scanning electron microscopy and transmission electron microscopy for reconstructed DA-LDH hybrid revealed that the sand-rose morphology of LDH layers developed during reconstruction provide DA molecules to be effectively separated in addition to the interlayer space of LDH layers. It was expected that the strong intermolecular interaction among DA moieties could be overcome by the in-situ development of sand-rose structured LDH particles through reconstruction reaction.

Poster Presentation : **MAT.P-484**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Organic Solvent Dispersable Silica Nanoparticles Bearing Linkers for Conjugation with Polymer Matrix

Jihyun Bang, Bongjin Moon*

Department of Chemistry, Sogang University, Korea

Silica nanoparticles (SNPs) are often used to reinforce optical coatings that require transparency due to hardness and particles size smaller than the wavelength of visible light. In these coatings, SNPs are dispersed in the polymer matrix, called polymer nanocomposites. The surface of the SNP is covered with hydrophilic silanol groups, and most of the polymers are hydrophobic. To mix the SNPs with the polymer solution, they need to be dispersed in organic coating solvents. Therefore, their silanol-rich hydrophilic surface should be modified to be hydrophobic. In our study, several functional groups (alcohol, aldehyde, epoxide, or oxetane, FGs) were introduced to make the SNPs surface hydrophobic and improve the homogeneity, allowing chemical immobilization with the polymer matrix. The goal of this study is to develop a more robust coating by introducing these FGs coated SNPs. These FGs are introduced during silica synthesis or added to the already synthesized SNPs.The desired SNPs are synthesized by sequential condensation of tetraethyl orthosilicate (TEOS) and trialkoxysilane in microemulsion. First, trialkoxysilanes with various FGs were prepared from the corresponding alkenes by hydrosilylation using Karstedt's catalyst. Then, SNPs having these FGs on the surface were synthesized from these trialkoxysilanes that are well dispersed in an organic solvent. These particles have a uniform size of about 50-90 nm confirmed from scanning electron microscope images. To determine the presence of epoxide groups on the surface, we treated the SNPs with fluorescent amines and measured the fluorescence. Epoxy-functionalized SNPs exhibited significant fluorescence compared to the unfunctionalized SNPs.

Poster Presentation : **MAT.P-485**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Selective or nonselective formation regarding numerous tiny-sized CNFs in carbon-based nonwoven fabrics and their electromagnetic shielding effectiveness

Hyun-Ji Kim, Sung-hoon Kim*

Department of Energy and Chemical Engineering, Silla University, Korea

Carbon microcoils (CMCs) were formed in carbon-based nonwoven fabrics (c-NFs) using C_2H_2 + SF_6 gas flow under thermal chemical vapor deposition system. By incorporating H_2 gas flow in C_2H_2 + SF_6 gas flow system, the selective hybrid formation of numerous tiny-sized carbon nanofibers (CNFs) in c-NFs, namely numerous tiny-sized CNFs formation only on the surfaces of individual carbon fibers (i-CFs) constituting c-NFs not on the surfaces of CMCs, was achieved. The cyclic process of SF_6 gas flow was performed by simply modulating SF_6 gas flow on and off in continuous cycles during the reaction. The samples with cyclic process can obviously give the nonselective hybrid formation tendency of numerous tiny-sized CNFs in c-NFs, namely tiny-sized CNFs formation on the surfaces of both i-CFs and CMCs. The morphologies, elemental components, and crystal structures of the samples were investigated. Based on these results, the detailed mechanisms were suggested for the selective or nonselective formation of tiny-sized CNFs formation in c-NFs. Furthermore, the electromagnetic wave shielding effectiveness (SE) values of the samples were investigated across the operating frequencies in the 8.0–12.0 GHz range. Among the previously reported total SE values, the presently measured values rank in top-tier. Although the electrical conductivity of native c-NFs was lowered by the hybrid formation, the total SE values for native c-NFs greatly increased following the hybrid formation. This dramatic improvement of total SE values was thought to be ascribed to the increased thickness of the nonwoven fabrics after the hybrids formation and the intrinsic characteristics of CMCs and the numerous cross-points of tiny-sized CNFs contributing to both the multiple reflections SE and the absorption SE in the fabric.

Poster Presentation : **MAT.P-486**
Material Chemistry
Exhibition Hall 1 THU 11:00~12:30

Electrically conducting two-dimensional polymers with band transport

Yeonsang Lee, Kimoon Kim[*]

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

Organic semiconductors have attracted a great deal of attention due to many practical advantages. Nevertheless, their poor conductivity and the absence of rigid electron pathway has been the source of its poor conductivity and hopping transport mechanism. Recently, pi-conjugated 2D polymers (C2Ps) have attracted considerable attention since they offer extended pi-conjugation along the second dimension. Nevertheless, the conductivity of the vast majority of C2Ps are either unknown or no match for inorganic counterparts, mainly attributed to rotatable single bonds within the layer that deters full-delocalization. Hence, it is essential to realize fully delocalized electron pathway throughout the material to achieve band transport. In that sense, C2Ps with fused aromatic linkage are idealized but largely unexplored owing to strong stacking and lateral dislocations between layers. Our research efforts were made to overcome such issues by introducing bulky pendants to prevent multi-layer stacking and increase the solubility of growth intermediates. The resulting C2P shows superior electrical conductivity after p-type doping, which is two order of magnitude higher than the previous record. Strikingly, band transport nature of the new C2P was revealed by Hall effect measurement with variable temperature down to 10 K. In this presentation, detailed synthetic strategies and experimental results will be covered.

Poster Presentation : **ELEC.P-487**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Self-organized hierarchically porous carbon coated on carbon cloth for high-performance freestanding supercapacitor electrodes

Myeongseok Jang, Yuanzhe Piao[1,*]

Graduate School of Convergence Science and Technology, Seoul National Univarsity, Korea
[1]*Graduate School of Convergence Science and Technology, Seoul National University, Korea*

In this work, a facile method is proposed for the fabrication of self-organized hierarchically porous carbon coated on carbon cloth. The method is based on the thermal treatment of potassium citrate gel, which is derived from mixture of citric acid and potassium hydroxide. The as-prepared porous carbon derived from citrate gel generally covers carbon cloth with fine morphological properties and the sample can be directly used as an electrode material for supercapacitor. In a three-electrode configuration, the optimized electrode exhibits a remarkable specific capacitance of 379.5 F/g at a current density of 1 A/g. In addition, a good cycle stability with capacity retention of 97% is achieved after 10,000 cycles at a current density of 10 A/g. Moreover, a symmetric supercapacitor is prepared by using the as-prepared electrode. The supercapacitor shows a high energy density of 0.7 mWh/cm3 at a power density of 4.9 mW/cm3 and good cycle durability and mechanical flexibility. The porous carbon material reported in this work shows potential as electrode for flexible all-solid-state supercapacitors.

Poster Presentation : **ELEC.P-488**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Molecular design for water-soluble polymer binder from nature-inspired molecules for high-performance silicon anodes in Lithium-ion batteries

Rajeev K K, Tae-Hyun Kim[1,*]

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

Silicon (Si) has attracted extensive interest as a promising high-energy anode material because of its superior theoretical capacity. However, the drastic volume expansion upon repeated lithiation/delithiation process results in the pulverization of the silicon electrode structure, poor electrochemical stability which hindered its practical applications. Many attempts have been made to mitigate this volume change issues, and one easy way is to develop polymeric binders that can accommodate silicon's volume changes, thereby improving the cycling stability of Si-based anodes. Herein, we synthesized chitosan-grafted gallic acid (CS-g-GA) as a water-soluble polymer binder in a simple, effective, and eco-friendly method. The overall results show that the presence of numerous hydroxyl groups from gallic acids would make strong hydrogen bonding interaction with SiNPs as well as the formation of irreversible internal crosslinking with gallol moieties in a 3D network structure. These effectively control the structural variations of SiNPs and maintain the structural integrity of the electrodes, resulting in higher electrochemical performances. The synthesis, characterization, and electrochemical properties of this newly developed polymer binder will be discussed in detail.Keywords: Chitosan-g-gallic acid, Polymer Binder, Silicon Anode, Lithium-Ion Batteries.

Poster Presentation : **ELEC.P-489**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Polymer Binder Materials in Conjunction with Ionic Liquid and Ceramic-based Flexible Sheet Electrolytes for All-Solid-State Batteries

Gaurav Thorat, Tae-Hyun Kim[1,*], Wonseok Jang[2]

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

All-solid-state batteries (ASSBs) are critical for increasing the energy density of modern lithium-ion batteries while also maintaining their safety. In this work, we report the fabrication of self-standing and electrochemically stable sheet-type composite solid-state electrolytes (SEs) with high ceramic loading using oxide ceramic powder, ionic liquid (IL), and polymers with distinct backbone structures, such as nitrile butadiene rubber (NBR), poly(vinylidene fluoride) (PVDF), and styrene-ethylene butylene styrene (SEBS). Over pristine ceramic-polymer electrolytes, the prepared SEs display higher ionic conductivity (~1.15 x 10^{-4} S cm^{-1}), reduced interfacial resistance, and electrochemical stability up to 5.5 V against Li^+/Li, thereby inheriting the merits of both ceramic and IL. The interfacial resistance between the SEs and the $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811) cathode was further reduced by direct incorporation of IL as a binder with polymer material in the cathode coating. The influence of IL on polymer binding properties is investigated using quantum chemical simulations. A Li/SEs/NCM811 solid-state cell shows excellent discharge capacity and suitable cycling stability after 50 cycles. This study clearly indicates that the utilization of such hybrid organic-inorganic system is an effective strategy for the commercialization of ASSBs.

Poster Presentation : **ELEC.P-490**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Carrageenan-based Polymer Binder for Si anode in Lithium Ion Battery

Wonseok Jang, Tae-Hyun Kim[1,*], Rajeev K K[2]

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

Silicon, which is naturally abundant and also has a high theoretical capacity, has been attracting much attention as a new anode material of the next generation LIB to replace graphite, currently used anode material in Li-ion battery (LIB). However, silicon has limitations due to its huge volumetric expansion and structural damage generated during the charging and discharging process, that leads to the loss of ion conduction pathways and reduced long-term durability. Polymer binders that have multiple functional sites to interact with Si have drawn recent attention as a solution to minimize these problems. In this study, Carrageenan has been extracted from seaweeds, and was used as a novel binder for Si anode. Among various forms, including Lambda, Iota, and Kappa, the Lambda-form of Carrageenan was successfully extracted, characterized, and investigated for its electrochemical properties in LIB.

Poster Presentation : **ELEC.P-491**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Synthetic Generality of Atomically Dispersed Pt Catalysts and Their Electrochemical Kinetics for the Chlorine Evolution Reaction

Taejung Lim, Jinjong Kim[1], Sang Hoon Joo[1,*]

School of Energy and Chemcial Engineering, Ulsan National Institute of Science and Technology, Korea
[1]*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

Electrochemical chlorine evolution reaction (CER) is a major anodic reaction for Cl2 production or on-site HClO generation. Although Ru-based mixed metal oxides have been used as commercial CER catalysts for the past half century, their oxide active sites also catalyze a parasitic oxygen evolution reaction (OER). Recently, we have developed a new class of CER catalysts based on atomically dispersed Pt–N4 sites on carbon nanotubes (Pt1/CNT). In this work, we demonstrated the synthetic generality of Pt–N4 sites for catalyzing CER and identified potential-dependent kinetics of Pt–N4 sites for CER. We prepared two types of Pt1/CNT catalysts using H2PtCl6·6H2O and ionic liquid via a bottom-up approach [Pt1/CNT(Cl)] and using Pt-porphyrin via a top-down approach [Pt1/CNT(P)]. Both the two Pt1/CNT catalysts comprised Pt–N4 active sites and exhibited similarly high CER activity (10 mA cm–2 @ 1.4 V vs. RHE), and ~100 % CER selectivity in OER-predominating 0.1 M NaCl electrolyte (pH 1), demonstrating the general nature of Pt–N4 as an effective catalytic site for CER. The analyses of Tafel slope, reaction order, and in situ X-ray absorption near edge structure (XANES) revealed pre-adsorbed Cl– before equilibrium potential of CER (1.36 V vs. RHE), indicating a unique CER behavior that commenced with Pt–Cl species. At low overpotential, the Pt1/CNT catalysts showed a reaction order (R) of ~1.8 and an average oxidation number (Ox.) of ~2.8 for CER evidencing the dominance of Volmer adsorption as the rate-determining step (RDS), which was clearly distinguished from the oxide-based CER catalysts (R ~ 1). As overpotential increases, CER over Pt1/CNT catalysts proceeds with decreasing reaction order and Ox. of ~3.9, indicating a switch to the Heyrovský discharge as the RDS.

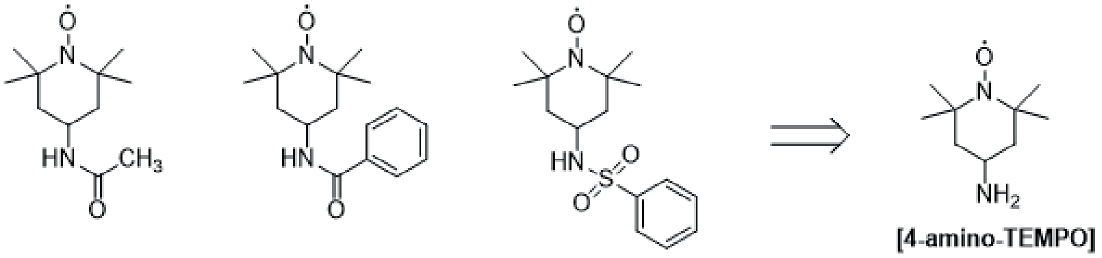
Poster Presentation : **ELEC.P-492**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Preparation of TEMPOL and Amino-TEMPO Derivatives: Tempol and Amino-tempo Adsorbed Li-TFSI Film for Fiber-Shaped Dye-Sensitized Solar cell.

Dongwook Jung, Myeonghwan Shin, Chuljin Ahn[1,*]

Chemistry, Changwon National University, Korea
[1]*Department of Biology and Chemistry, Changwon National University, Korea*

Fiber-shaped solar cells (FSCs) have attracted academically and industrially intense interest due to their light weight, flexibility, weavability, and wearability. FS-DSSC using Li-TFSI film as a quasi-solid-state electrolyte with both traditional electrolyte and TEMPOL and amino-TEMPO electrolyte were first designed. The TEMPOL and amino-TEMPO derivatives as electrolyte were prepared conveniently.



[ATA] [ATBZ] [ATBS] [4-amino-TEMPO]

Poster Presentation : **ELEC.P-493**

Electrochemistry

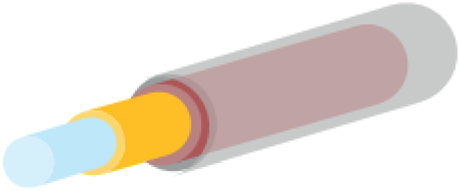
Exhibition Hall 1 THU 11:00~12:30

Preparation of Oxo-TEMPO Derivatives : Oxo-TEMPO Adsorbed Li-TFSI Film for Fiber-Shaped Dye-Sensitized Solar Cell.

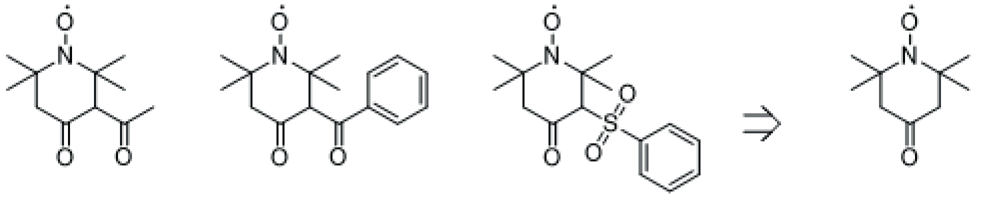
Myeonghwan Shin, **Dongwook Jung**[1], **Chuljin Ahn**[2,*]

chemistry, Changwon National University, Korea
[1]*Chemistry, Changwon National University, Korea*
[2]*Department of Biology and Chemistry, Changwon National University, Korea*

Fiber-shaped solar cells (FSCs) have attracted academically and industrially intense interest due to their light weight, flexibility, weavability, and wearability. FS-DSSC using Li-TFSI film as a quasi-solid-state electrolyte with both traditional electrolyte and Oxo-TEMPO electrolyte were first designed. The Oxo-TEMPO derivatives as electrolyte were prepared conveniently.



HSE + Li-TFSI film
- HSE Dipping
- Li-TFSI film wrapping
- Dipping of OTA, OTBZ, OTBS,
- HSE dipping



[OTA] [OTBZ] [OTBS] [Oxo-TEMPO]

Poster Presentation : **ELEC.P-494**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

In situ synthesis of Ni single atom catalyst on glassy carbon electrode for enhanced electrochemical CO_2 reduction reaction

Dongho Seo, Ki Min Nam*

Department of Chemistry, Pusan National University, Korea

Electrochemical reduction reaction of carbon dioxide (CO_2RR) provides a useful source of valued hydrocarbons, and it is a promising approach to reduce carbon dioxide levels. However, poor product selectivity is still a major obstacle to the development of electrochemical CO_2RR. In addition, the stability of the catalysts during electrolysis is of great meaningful. Here we report facile synthesis of glassy carbon electrode on an alumina plate, and consecutive synthesis of a Ni single atom catalyst on the glassy carbon electrode (Ni SAC-GC). The Ni SAC-GC electrode exhibited excellent activity for electrochemical CO_2RR with especially high selectivity, achieving high faradaic efficiency (FE) over 90% for carbon monoxide in the potential range from −0.65 V to −1.35 V and gives a maximum FE of 95% at −1.05 V. In addition, the Ni SAC-GC electrode was highly stable, indicating strong interaction between Ni SAC and the GC substrate. We are expected to shed new light on the development of robust electrode that are suitable for industrial application.

Poster Presentation : **ELEC.P-495**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Optimizing Mg^{2+}/Al^{3+}-Doping of NCM811 Cathode for Enhanced Electrochemical and Structural Stability

Haein Jeong, Hyun Deog Yoo[1,*]

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

Lithium-ion batteries (LIBs) have wide applications in various fields due to their low cost and high performance. Recently, many studies have been conducted to achieve high energy density required for electric vehicles (EVs) and hybrid electric vehicles (HEVs). Among cathode materials, Ni-rich $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811) is a promising cathode material because of its excellent electrochemical performance and cost effectiveness due to the low cobalt content. However, NCM811 has poor cycling stability mainly because of the facilitated side reactions and structural instability by the increased portion of nickel ions. Herein, we doped Mg^{2+} and Al^{3+} into NCM811, and studied the effects of doping level on the electrochemical and structural stability. After studying the physicochemical and electrochemical properties of NCM811, we performed *in-operando* XRD to analyzed the real-time structural change during the cycling. Overall, doped NCM811 represented enhanced structural and thermal stability, exhibiting superior electrochemical performances compared to the pristine NCM811. The doped samples showed slightly lower initial discharge capacity than the pristine NCM811; however, the long-term capacity retention of doped NCM811 samples was superior than the pristine NCM811. The *in-operando* XRD analysis revealed that the Mg^{2+}-doping mitigated the abrupt decrease in the *c*-axis parameter due to the H2-H3 phase transition at the end of the charging. Thus, optimized amount of Mg^{2+} and Al^{3+} doping successfully improved the structural and electrochemical stability of the Ni-rich NCM811 cathodes.

Poster Presentation : **ELEC.P-496**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Electrochemically Generated Mesopores and Residual Oxygen for Improved Activity of Silver Electrocatalysts

Sangram Keshari Mohanty, Hyun Deog Yoo[1,*]

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

The development of stable and efficient electrocatalysts is of key importance for the establishment of a sustainable society. The activity of a metal electrocatalyst is determined by its electrochemically active surface area and intrinsic activity, which can be increased using highly porous structures and heteroatomic doping, respectively. Herein, we propose a general strategy of generating mesopores and residual oxygen in metal electrocatalysts by reduction of metastable metal oxides using Ag_2O_3 electrodeposited onto carbon paper as a model system and demonstrating that the obtained multipurpose porous Ag electrocatalyst has high activity for the electroreduction of O_2 and CO_2. The presence of mesopores and residual oxygen is confirmed by electrochemical and spectroscopic techniques, and quantum mechanical simulations prove the importance of residual oxygen for electrocatalytic activity enhancement. Thus, the adopted strategy is concluded to allow the synthesis of highly active metal catalysts with controlled mesoporosity and residual oxygen content.

Poster Presentation : **ELEC.P-497**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Synthesis of hollow columnar nanostructures of bimetallic phosphides as electrocatalysts for oxygen evolution reaction

Jihye Son, Siva Kumar Ramesh, Jinkwon Kim[*]

Department of Chemistry, Kongju National University, Korea

In this presentation, synthesis, structural characterizations, and electrochemical catalytic performances of hollow nanostructures of transition metal selenides will be demonstrated. Hollow nanostructures of transition metal selenides were synthesized from a reaction of $[Fe(CN)_6]^{3-}$ or $[Co(CN)_6]^{3-}$ anions with $Ni_2(BDC)_2(DABCO)$ template MOF. Uniform hexagonal column-shaped $Ni_2(BDC)_2(DABCO)$ nano crystals were synthesized under an ultrasonic condition. Hollow-structured $M_x\{Ni(CN)_6\}_y$ prussian blue analogues (MNi-PBAs) were produced by a slow etching process $Ni_2(BDC)_2(DABCO)$ nanocrystals with a small amount of acid while simultaneously reacting with $[M(CN)_6]^{3-}$ (M = Ni, Co) ions. Selenization, Phosphidation, and oxidation of MNi-PBAs were conducted to obtain NNiP-FeP, $NiSe_2$-Fe_3Se_2, $NiCo_2O_4$, NiP_2-Co_2P, Ni_3Se_4-$CoSe_2$ hollow nanostructures. The results of various structural characterizations such as XRD, XPS, SEM and electrocatalytic performances of these nano materials will be presented.

Poster Presentation : **ELEC.P-498**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

LiX Electrolyte Additive for High-Performance Anode-free Lithium Metal Battery

Amol Bhairuba Ikhe, Myoungho Pyo*

Department of Printed Electronics Engineering, Suncheon National University, Korea

Lithium metal batteries are the key to achieving high specific energy for the electrification of aviation and transportation. Anode-free lithium metal batteries (AFLMB) are lithium metal batteries with no excess lithium metal with the highest possible specific energy density. The AFLMB will be a cheaper, safer, and easy cell fabrication process in comparison with that of the current lithium-ion battery technology. However, the practical implementation of an AFLMB is hampered by dendrite formation and low coulombic efficiency. These challenges are mainly raised due to the non-uniform lithium plating and unstable SEI layer formation on the bare copper substrate. The consumption of lithium during each cycle to reform SEI causes low coulombic efficiency, which resulted in low cyclic stability. Therefore, there is a tremendous need to grow uniform lithium plating with stable SEI to archive a high stability AFLMB. Herein, to archive high cyclic stability in anode-free cells, we have focused on the stabilization of an SEI by using an electrolyte additive. The X mM of LiX was intentionally added to the electrolyte, which not only derives a stable SEI but also gives a uniform lithium plating on the copper substrate. Detailed electrochemical and spectroscopic investigations on the lithium plating/stripping are underway.

Poster Presentation : **ELEC.P-499**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Metal-Organic Framework-Derived NiSe2-FeSe Double-Shelled Hollow Polyhedrons for Efficient Electrocatalytic Oxygen Evolution Reaction

Siva kumar Ramesh, Jinkwon Kim[1,*]

Chemistry, Kongju National University, Korea

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

Development of hollow structured hybrid electrocatalyst is significantly essential for efficient and low-cost electrochemical water splitting systems. In this work, $NiSe_2$-FeSe double-shelled hollow polyhedrons (DHPs) is synthesized via a MOF-based self-templating approach for efficient oxygen evolution reaction (OER) in alkaline solutions. First, MIL-88A was converted to NiFe-LDH DHPs by etching and coprecipitation, followed by selenization treatments to prepare $NiSe_2$-FeSe DHPs. Benefiting from the synergetic effect of heterostructure selenide composition and double-shelled hollow structure, $NiSe_2$-FeSe DHPs have a high specific surface area and superior electrocatalytic OER performance. The as-prepared $NiSe_2$-FeSe DHPs exhibit a low overpotential, a small Tafel slope, and excellent stability for 24 h. Post-XPS and SEM measurement of $NiSe_2$-FeSe DHPs indicates the robust nature of the catalyst.

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **ELEC.P-500**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Preparation of Porous Carbon Nanofibers with Cobalt for Electrochemical Performance

Jihee Choi, Donghee Kim, Sang Eun Hong, Kuk Ro Yoon*

Chemistry, Hannam University, Korea

In the recently years, carbon electrode materials for supercapacitors have been widely investigated, because of its high conductivity, lower resistance and good stability. The porous carbon nanofibers (PCNFs) have been actively developed as an indispensable candidate for electrode materials of supercapacitors. The PCNFs were prepared via electrospinning ternary PAN/N, N'-dimethylformamide (DMF)/ tetrahydrofuran (THF) and using uniformed CaCO3 nanoparticles as template. The obtained modified porous carbon nanofiber with cobalts attain high specific surface area without physical and chemical activation. Consequently, electrode material combines the advantages of mesoporous structure and high specific surface area and has exhibited excellent capacitance performance. Also, the physicochemical characteristics were evaluated by Optical microscope, FE-SEM, FE-TEM, EDS, FT-IR, and Cyclic voltammetry analyses.

Poster Presentation : **ELEC.P-501**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Study of photoelectrochromic device performance comparing different methyl group positioning on salicylic acid sensitizers

Seok In Lee, Chi-Hwan Han[1,*]

Department of Chemistry, Korea University, Korea

[1]*New and Renewable Energy Division, Korea Institute of Energy Research, Korea*

Photoelectrochromic device(PECD), which is an integrated device of photoanode and electrochromic cathode do not need any external power source to regulate the transmittance. Most of the previous researches on PECDs have used N719 dye as a sensitizer of photoanode however N719 has drawbacks of slight red tint and long-term stability.Recently Saad et. al reported the utilization of a ligand, Methyl Salicylic Acid to sensitize the TiO_2 layer in PECD. It has been reported that PECD to which methyl salicyclic acid is applied as sensitizer has advantages such as low price, fast color change, and improved long-term stability. Depending on the position of the methyl, methylsalicyclic acid exists as 3-, 4-, 5-, 6-methylsalicyclic acid.In this study, we have applied various methylsalicyclic acid to PECD and compared the performance with the difference of methyl positioning. The changes in transmittance for coloration, kinetics like coloration speed and bleaching speed, repeatability of the color change have been checked and compared.

Poster Presentation : **ELEC.P-502**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Reverse Engineering Applied to the study on MoS_2's redox property.

Kyunghwan Chai, **Mijeong Kang**[1,*]

Department of Nano Mechatronics Engineering, Pusan National University, Korea
[1]*Department of Optics and Mechatronics Engineering, Pusan National University, Korea*

Oxidative stress causes various diseases such as Parkinson's disease. A lot of research has been conducted to reduce oxidative stress, and the treatment with antioxidants is one of the major methods. However, there are limitations in using common antioxidants. Organic antioxidants, for example, are sensitive to pH changes, resulting in poor efficiency, and can scavenge specific ROS. Therefore, it is necessary to develop next-generation inorganic antioxidants. MoS_2 has been recently emerged as a good antioxidant material. MoS_2, however, has both antioxidant and prooxidant properties, and no research has been conducted to comprehensively understand the its redox properties and the underlying mechanism. The conventional method uses end-point assays and provide limited information on the redox properties and mechanism of MoS_2. In this study, we used adjustable electrical potential and electrochemical mediators to study the various aspects of the antioxidant and prooxidant mechanism of MoS_2. MoS_2 showed higher levels of antioxidant capabilities than organic antioxidants, and we expect that MoS_2 can provide a variety of interesting antioxidant performances.

Poster Presentation : **ELEC.P-503**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Water-in-salt electrolyte enabled molecular anion-shuttling battery

Arpan Samanta, Myoungho Pyo[1,*]

Department of Advanced components and Materials Engineering, Suncheon National University, Korea
[1]*Department of Printed Electronics Engineering, Suncheon National University, Korea*

The quest for the development of next-generation energy storage systems beyond Li-ion batteries (LIBs) has been gained more and more popularity as LIBs is being approaching the energy limit. One candidate is a rocking-chair-type “molecular ion battery” in which a molecular ion, instead of lithium ion, works as a charge carrier. To build such a molecular ion battery system, the concept of replacing conventional inorganics by redox active organics as electrode material has been proposed due to their high structural designability and tunability. However, capacity fading and poor cycling stability stemming from the dissolution of the organic active compounds in common electrolytes is remained one of the major challenges of the molecular ion battery. Herein, we demonstrate a molecular anion-shuttling battery based on cross-linked viologen (CLV) derivative as negative electrode material that releases and receives anions during the charge–discharge process. Furthermore, a highly concentrated aqueous electrolyte (> 21 m) which is also known as water-in-salt electrolyte (WiSE) has also been introduced to circumvent the dissolution problem of the organic electrode. WISEs have attracted widespread attention due to their non-flammability, environmental friendliness, and wider electrochemical stability window than conventional dilute aqueous electrolytes. It is well known that almost all of the water molecules participated in the solvation of salt-metal ions in WiSE, and the absence of free water reduces the chance of the dissolution of CLV at anode; results in improved capacity and cycling stability. The work is in progress.

Poster Presentation : **ELEC.P-504**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Development of Ion-Selective Electrodes for Soil Nutrients

SeongJun Hong, Seonghyun Hong, Yang-Rae Kim*

Department of Chemistry, Kwangwoon University, Korea

Recently, there is a worldwide interest in the development of direct and fast analysis of soil nutrients. Soil nutrient analysis focuses on the measurement of specific elements, such as nitrogen (N), phosphorus (P), and potassium (K). Because they are essential nutrients for crop growth, it is crucial to control quantifying the N, P, and K inputs in farming soils for high yields and high-quality crop growth. Typical methods for soil analysis include colorimetry, atomic spectroscopy, flame photometry, and spectrophotometry. However, some of them require pretreatments and laboratory facilities. Also, some cannot simultaneously measure N, P, and K. In comparison, an electrochemical ion-selective electrode (ISE) is an appealing technique to monitor soil nutrients. It does not require a sophisticated experimental setup and can be deployed directly into the soil for elemental analysis. In addition, ISE can be miniaturized and highly integrated with electronic circuits. Also, it allows multiple detections and rapid measurement with high reliability and precision.In this study, several ion-selective membranes were fabricated with high sensitivity towards each N and K. These membranes are employed to develop ISEs. Their performance, such as sensitivity, selectivity coefficient, and detection range, has been investigated and compared with commercialized ISE.This work was carried out with the support of Cooperative Research Program for Agriculture Science and Technology Development (Project No. PJ015725032021) Rural Development Administration, Republic of Korea.

Poster Presentation : **ELEC.P-505**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Effects of Shape and Hydriding for Palladium Nanocatalyst toward Oxygen Electroreduction Reaction

Mrinal kanti Kabiraz, Jeonghyeon Kim, Sang-Il Choi[1,*]

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

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

Proton exchange membrane fuel cells (PEMFCs) is considered one of the cleanest and most efficient energy conversion device. Oxygen reduction reaction (ORR) occurring at the cathode of PEMFCs has been acknowledged as the primary bottleneck due to the sluggish electron-transfer kinetics that limits the cell efficiency. While platinum (Pt) based catalysts are regarded as the most active catalyst toward the ORR, palladium (Pd) has also drawn significant attention as potential electrocatalysts in acidic and alkaline media. This study represents Pd octahedra and cubes enclosed by {111} and {100} facets, respectively, and their hydride forms (PdH) as model catalysts, which were synthesized to probe the shape and composition effects on ORR. The hydriding effect improved the ORR performance on the PdH octahedra compared with Pd octahedra. On the other hand, PdH cubes showed a decrement in ORR activity compared to Pd cubes. The opposite trend of the hydriding effect in relation to shape was explained with Sabatier's principle, where the optimal OH binding strength of nanocatalyst governs ORR activity.

Poster Presentation : **ELEC.P-506**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Simple Electrochemical Detection of Porphyromonas gingivalis in Saliva for Initial Diagnosis of Periodontitis

Seonhwa Park, Haesik Yang[*]

Department of Chemistry, Pusan National University, Korea

Indirect detection of Porphyromonas gingivalis in saliva, based on proteolytic cleavage by gingipain (Arg-gingipain), has traditionally been used for initial diagnosis of periodontitis. However, the traditional detection method using a colorimetry divides the concentration of P. gingivalis into positive, weakly positive, and negative only. The electrochemical detection in saliva is difficult because saliva contains various interfering electroactive species. Here, we report electrochemical biosensor for sensitive and simple detection of P. gingivalis in saliva. An electrochemical active species, 4-aminophenol (AP), is liberated by the proteolytic reaction between a peptide substrate (Glycine-proline-arginine conjugated wit AP) and a gingipain which is a trypsin-like protease in the outer membrane of P. gingivalis. The electrochemical signal of AP was amplified by electrochemical-chemical (EC) redox cycling involving a indium-tin oxide electrode partially modified with multi-well carbon nanotubes, AP, and tris(2-carboxyethyl)phosphine, and the electrochemical charge signal was corrected using the initial charge obtained before an incubation period. The calculated detection limit for P. gingivalis in artificial saliva was 5 × 105 CFU/mL, and the concentration of P. gingivalis in human saliva could be measured. The developed biosensor can be used as an initial diagnosis method to distinguish between healthy people and patients with periodontitis.

Poster Presentation : **ELEC.P-507**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Simple β-Galactosidase-Induction-Based Electrochemical Detection of *Escherichia coli*

Jungwook Kwon, Haesik Yang[*]

Department of Chemistry, Pusan National University, Korea

Escherichia coli (*E. coli*) is recognized as an indicator of fecal bacterial contamination, and the induction of intracellular β-galactosidase (Gal) is commonly used for sensitive and selective *E. coli* detection. However, this method requires a simple procedure to ensure that the Gal substrate and product are highly permeable through the *E. coli* membrane, making it unsuitable for simple point-of-care detection. Here, we report a sensitive electrochemical method for *E. coli* detection that does not require a permeabilization process. Intracellular Gal expression is increased via induction by isopropyl-β-D-thiogalactopyranoside (IPTG). 4-Methoxyphenyl-β-D-galactopyranoside (MPGP) and 4-methoxyphenol (MP) are used as the highly cell-permeable Gal substrate and product, respectively. Externally-added tyrosinase (Tyr) converts MP into electrochemically active 4-methoxycatechol, which is then electrochemically oxidized via electrochemical-chemical redox cycling involving an electrode, 4-methoxycatechol, and tris(2-carboxyethyl)phosphine. The presence of MPGP during the induction of intracellular Gal led to amplified MP production. The results of four different detection methods using three Gal substrates (MPGP, phenyl-β-D-galactopyranoside, and 4-aminophenyl-β-D-galactopyranoside) were compared. The detection limit for both drinking water and tap water spiked with *E. coli*, obtained following a 2-h-long IPTG treatment and 5-min-long Tyr reaction, was ~2×10^3 colony-forming units (CFU)/mL, indicating that this method can be applied to monitoring *E. coli* contamination in water samples. Importantly, the present method does not require the electrode modification, affinity binding, washing, and filtration steps.

Poster Presentation : **ELEC.P-508**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Boosting Electrochemical Immunosensing Performance by Employing Acetaminophen as a Peroxidase Substrate

Jihyeon Kim, Haesik Yang[1,*]

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

In horseradish peroxidase (HRP)-based electrochemical immunosensing, an appropriate HRP substrate needs to be chosen to obtain a high electrochemical signal-to-background ratio. This is limited by the unwanted electrochemical reduction of H_2O_2, oxidation of the substrate, and the slow electrochemical reduction of the product. Herein, we report acetaminophen (AMP) as a new HRP substrate that allows for highly sensitive immunosensing. Electrochemical behavior and immunosensing performance using AMP are compared with those using the most popular HRP substrate, hydroquinone (HQ). To maintain a high electrocatalytic activity even at an electrode modified with an immunosensing layer, an indium tin oxide electrode partially modified with reduced graphene oxide is employed. AMP allows for a higher signal-to-background ratio than HQ, because the formal potential of AMP is 0.28 V higher than that of HQ and the redox reaction of AMP is as reversible as that of HQ, resulting in a lower detection limit in a sandwich-type immunoassay using AMP for thyroid-stimulating hormone detection. The calculated detection limit is ~0.2 pg/mL. The use of AMP as an HRP substrate is especially promising for highly sensitive electrochemical immunoassays.

Poster Presentation : **ELEC.P-509**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Methionine assisted electrodeposition of copper cobalt bi-metallic nanostructures: A stable electrode material for highly sensitive glucose detection

Jiwon Kim, Viswanathan Perumal[1], Kyuwon Kim[1,*]

Chemistry, Incheon National University, Korea

[1]Department of Chemistry, Incheon National University, Korea

In the present investigation, we are presenting a biomolecule assisted electrodeposition of copper-cobalt bimetallic nanostructures for highly sensitive glucose detection. Usually, as electrodeposited Cu-Co films on ITO electrodes are not stable, they easily peel off from the electrode surface. To address this issue many strategies being followed. Especially, for very smooth surfaced glass-based electrodes like ITO and FTO, high temperature calcination after electrodeposition is the main strategy to form stable modified electrodes. But in the present work, we have found a very simple and facile method to make very stable electro-deposited films on the ITO electrode using thiol-functionalized amino acid, methionine. Methionine was found to play multiple roles like structure directing agent, stabilizing agent and also alters the composition of electrode films. Further, the prepared electrodes were succefully utilized for the glucose electro-oxidation and sensing. The designed glucose sensor shows very high sensitivity and selectivity towards glucose with low detection limit. The electroanalytical performances were superior to many already reported results.

Poster Presentation : **ELEC.P-510**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Magneto-Plasmonic Nano-Heterostructures Based on Prussian Blue-Silver Composite: An Efficient Electrochemical Probe for the Identification of Nitrite Milk-Tainting

Viswanathan Perumal, Dohun Lee[1], Kyuwon Kim*

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

Magneto-plasmonic nanocomposites are very attractive and emerging multifunctional materials find application in many fields. Replacing the pure inorganic magnetic core with a molecule-based magnet (like Prussian blue (PB)) and plasmonic gold with low-cost plasmonic material (like silver and copper) and exploring their electrocatalytic properties would be an interesting and new research direction. In the investigation, the PB nanostructure is electrodeposited on the silicate matrix modified electrode surface followed by Ag heterostructure was coated on the PB surface through galvanic replacement reaction with the assistance of PB as a sacrificial template and glutamine to endow the magneto-plasmonic structure (PB-Ag). The plasmonic Ag coating on the magnetic PB structures play multiple roles such as protecting PB nanostructure, increase their stability, increasing the conductivity of composite, increasing the electrocatalytic and sensing activity of the composite. The prepared magneto plasmonic nanocomposite was directly applied for electrocatalysis and sensing towards nitrite ions. Interestingly, the material exhibits superior sensing properties towards nitrite with excellent selectivity in comparison with already reported results.

Poster Presentation : **ELEC.P-511**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Diaphorase-Catalyzed Formation of a Formazan Precipitate and Its Electrodissolution for Sensitive Parathyroid Hormone Detection

Gyeongho Kim, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

Catalytic precipitation and subsequent electrochemical oxidation or reduction of a redox-active precipitate has been widely used in electrochemical biosensors. However, such biosensors often do not allow for low detection limits due to a low rate of precipitation, nonspecific precipitation, loose binding of the precipitate to the electrode surface, and insulating behavior of the precipitate within a normal potential window. In this presentation, we report an ultrasensitive electrochemical immunosensor for parathyroid hormone (PTH) detection based on DT-diaphorase (DT-D)-catalyzed formation of an organic precipitate and electrochemical oxidation of the precipitate. In the present study we found that DT-D can be used as a catalytic label in precipitation-based affinity biosensors because DT-D catalyzes fast reduction of 3-(4,-5-dimethylthiazo-2-yl)-2,5-diphenyltetrazolium bromide (MTT) to MTT-formazan precipitate; the MTT reduction does not occur in the absence of DT-D; and a high electrochemical signal is obtained at low potentials during electrodissolution of MTT-formazan precipitate. The immunosensor is fabricated using a silane copolymer-modified ITO electrode surface that is suitable for both efficient and strong adsorption of MTT-formazan precipitate. When the enzymatic MTT-formazan precipitation and subsequent MTT-formazan electrodissolution is applied to a sandwich-type immunosensor, PTH can be detected over a wide range of concentrations with a very low detection limit (~1 pg/mL) in artificial serum. The measured concentrations of PTH in clinical serum samples showed high similarity with those obtained using a commercial instrument.

Poster Presentation : **ELEC.P-512**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Cellulose nanofiber derived carbon and reduced graphene oxide co-supported LiFePO4 nanocomposite for high-performance lithium-ion battery cathode

Seungman Park, Yuanzhe Piao[1,*]

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

Over the past few years, tremendous efforts have been focused on the development of lithium-ion batteries (LIBs) used in portable electric devices, hybrid electric vehicles (HEVs), and electric vehicles (EVs) because of their long cycle stability and high energy density. Among the various cathode materials, lithium iron phosphate ($LiFePO_4$, LFP) has been attracted as a promising candidate because of its low cost, naturally abundant, low toxicity, superior thermal stability, and excellent safety performance. However, intrinsically low lithium-ion diffusion coefficient and low electric conductivity are inhibiting the high-rate performance and the commercialization of HEVs and EVs. In this work, cellulose nanofiber (CNF) derived carbon and reduced graphene oxide co-supported LFP nanocomposite was prepared by thoroughly mixing CNF with LFP first, followed by mixing again with graphene oxide (GO) to make well dispersed LFP nanoparticles anchored on graphene oxide, finally heating under an inert atmosphere. The ultrathin CNF was used as not only a carbon source but also an adhesive agent which can attach the LFP nanoparticles to the graphene sheets leading to reduce contact resistance. Consequently, this nanocomposite exhibited good rate performance (discharge capacity of 168.9 mA h/g at 0.1 C, and 90.3 mA h/g at 60 C) and long-term cycle stability (~91.5% of initial capacity at 10 C after 500 cycles)

Poster Presentation : **ELEC.P-513**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis and electrochemical performance of (100-x)Li_6PS_5Cl-x$LiNbO_3$ solid electrolyte for all solid state lithium batteries

Ji un Cho, Kwang Sun Ryu*

Department of Chemistry, University of Ulsan, Korea

Lithium-ion batteries (LIBs) have been widely applied to various electronic devices and electric vehicles in our society. However, the safety concern in conventional LIBs which originated from the usage of flammable organic liquid electrolyte and the limitation of energy density make it difficult for their further application. All-solid-state lithium batteries (ASSLBs) with solid electrolyte to replace the liquid electrolyte have attracted great attention as next-generation batteries because of the good thermal stability and high energy density. Among available solid electrolytes, one of the sulfide solid electrolytes, Li-argyrodite Li_6PS_5X (X = Cl, Br, and I) has a wide electrochemical window and good mechanical deformability. The ionic conductivity of Li_6PS_5X (X = Cl, Br, and I) is 10^{-6} S cm^{-1} for Li_6PS_5I, 10^{-3} S cm^{-1} for Li_6PS_5Cl, and Li_6PS_5Br has intermediate conductivity. The ionic conductivity of Li_6PS_5X (X = Cl, Br, and I) has been improved using various approaches.In this work, by introducing $LiNbO_3$ as an additive for Li_6PS_5Cl solid electrolyte, we enhanced the ionic conductivity of Li_6PS_5Cl. The $LiNbO_3$ doped/mixed Li_6PS_5Cl solid electrolytes were prepared by high energy ball milling process and subsequent heat treatment. The crystal structures of the synthesized electrolytes were characterized using powder X-ray diffraction (XRD). The surface morphology and element analysis of the electrolytes were performed on field emission scanning electron microscope (FE-SEM) with energy dispersive X-ray spectroscope (EDS). The ionic conductivities of the prepared solid electrolytes were measured by electrochemical impedance spectroscopy (EIS). The synthesized 96Li_6PS_5Cl-4$LiNbO_3$ solid electrolyte exhibited high ionic conductivity (4.29 mS cm^{-1}) at room temperature compared to the pure Li_6PS_5Cl solid electrolyte (3.23 mS cm^{-1}). Furthermore, cyclic voltammetry measurement and DC cycling stability test were performed to confirm the electrochemical stability of the prepared solid electrolytes.

Poster Presentation : **ELEC.P-514**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Facile one-step synthesis of trimetallic N-doped CoNiFe amorphous with excellent oxygen evolution reaction

Anh.T.N Nguyen, Min-ji Kim[1], Jun Ho Shim[1,*]

Department of Chemistry, Daegu University, Vietnam
[1]*Department of Chemistry, Daegu University, Korea*

Hydrogen is considered as one of the promising clean fuels and important part of the future of renewable energy that can address global energy demand and environmental issues. However, one of the major problems for hydrogen economy is its clean production because a great majority of current used hydrogen is produced mainly by fossil fuel via the steam reforming process, from which carbon dioxide also generated as the byproduct. Therefore, a great deal of efforts has been made to produce hydrogen from water electrolysis, which is an environmentally clean, potentially cost-effective and renewable source of hydrogen. At present, noble ruthenium oxide and iridium oxide materials are regarded as the most effective OER electrocatalysts, while they are not available for the large-scale application due to high cost and their low natural abundance. Over the past decades, a tremendous progress has been observed in transition metal-based electrocatalysts such as metal oxide, metal hydroxide, metal phosphide, metal chalcogenides that can be promising alternative materials with good OER performances for electrochemical water splitting. In this presentation, a trimetallic nitrogen-doped CoNiFe amorphous (N-CoNiFe) is developed for the first time using a facile and practical strategy co-precipitation method in the presence of ethanolamine. The prepared N-CoNiFe catalyst showed remarkable electrocatalytic activity for OER, with the overpotential of 329 mV at 10 mA cm-2 in 1.0 M KOH and a Tafel slope of 60.1 mV dec-1. The enhanced OER performance is attributed to the following reasons: (1) the synergistic effect between different metal sites; (2) amorphous material with a large number of active sites and improve intrinsic activity; (3) nitrogen doping boosts the electrical conductivity of CoNiFe system.

Poster Presentation : **ELEC.P-515**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

MoS_2@FeNC Nanospheres for Oxygen Reduction, Hydrogen Evolution Reaction and Detection of H_2O_2 from Living Cells

Khatun a Jannath, Deog Su Park[1], Yoon Bo Shim[2,*]

Molecular Science Technology, Pusan National University, Bangladesh
[1]*Biophysio Sensor Technology, Pusan National University, Korea*
[2]*Department of Chemistry, Pusan National University, Korea*

Carbon materials with multifunctional catalytic activity and superior stability is essential for their applications as electrocatalysts. We report synthesis and characterization of a vertically aligned MoS_2 nanosheet-anchored FeNC nanospheres (MoS_2@FeNC). The hybrid structure of the nanosphere exhibits robust bifunctional catalytic activity towards ORR, HER and detection of H_2O_2 released from living cells. MoS_2 nanosheets with expanded interlayer spacings are vertically grown on Fe and N doped carbon (FeNC) particles to form MoS_2@FeNC hierarchical nanospheres by a simple hydrothermal process followed by pyrolysis at 800 °C. MoS_2@FeNC exhibits a superior oxygen reduction reaction performance with a half wave potential of 0.879 V (vs RHE) and a small Tafel slope of 61 mV/dec, which is better than that of benchmark Pt/C (0.864V and 63 mV/dec) with excellent methanol tolerance and stability in 0.1 M KOH. The activity of MoS_2 towards hydrogen evolution reaction is also impressive with a small overpotential of 162 mV (vs RHE) at 10 $mAcm^{-2}$ and a Tafel slope of 66 mV/dec in alkaline condition. Additionally, the electrocatalyst exhibits enhanced analytical performance for the detection of H_2O_2 from A549 cells with a detection limit of 200 nM.

Poster Presentation : **ELEC.P-516**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

N-doped Carbon Framework-based Electrocatalysts for Oxygen Reduction Reaction by NH_3 Activation

<u>Sungjun Heo</u>, Je Seung Lee*, Sung Yul Lim*

Department of Chemistry, Kyung Hee University, Korea

Pt-group metal electrocatalysts have been the most efficient catalysts for the oxygen reduction reaction (ORR). However, due to the high cost of noble metals, the development of non-noble metal-based or metal-free electrocatalysts has been investigated for decades. Here, we report metal-free, N-doped mesoporous nanocarbon electrocatalysts with highly ordered nanochannels for the ORR. N-containing species are introduced in the carbon frameworks through heat treatment under NH_3 atmosphere for activation. During this thermal activation process, surface area increases while maintaining the mesopore in the carbon frameworks. As a result, N-related chemical species by NH_3-treatment at high temperature significantly improve the ORR performance in alkaline electrolyte. Moreover, electrocatalytic activity in ORR are retained during 40,000 cycles of the accelerated stability test (AST). During the AST, the chemical structural changes were studied by X-ray photoelectron spectroscopic (XPS) analysis. The correlation between the ORR activity and active sites, originating from pyridinic N and graphitic N, is identified from this XPS analysis.

Poster Presentation : **ELEC.P-517**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Modified the Morphology of One-dimensional Au and Fe Complex Photoanode with Ni doping for Enhancing the Efficient Oxygen Evolution Reaction

Sohyun Kang, Jaebeom Lee[*]

Chemistry, Chungnam National University, Korea

For the generation of environmentally friendly energy sources, hydrogen production through electrochemical water-splitting ($2H_2O \rightarrow 2H_2 + O_2$) has been developed. Integrating earth-abundant active oxygen evolution catalysts (OECs) with diverse photoanodes is very important to realize efficient photoelectrochemical (PEC) water splitting. The hematite (Fe_2O_3) is a suitable candidate for the PEC water splitting due to its well-suited band structure, stability in chemical and thermodynamically, and availability. However, the rapid charge recombination and the sluggish water oxidation kinetics are still key drawbacks that limit the PEC water splitting efficiency of Fe_2O_3. Herein, we modify the surface alignment of the maghematite nanowires using magnets. The property of maghematite which we made has a superparamagnetic property. This is the reason how the alignment is easily controlled. The catalyst is composed of the core@shell structure. Moreover, the other exceptional property is the edge of the shell is naked, making the gold appear on the surface. Benefited from the accelerated OER kinetics and low overpotential with nickel doping, the resultant heterojunction interface possesses better visible light absorption, enhanced photocurrent density, and better stability than bare hematite and semi-FeOOH photoanodes.

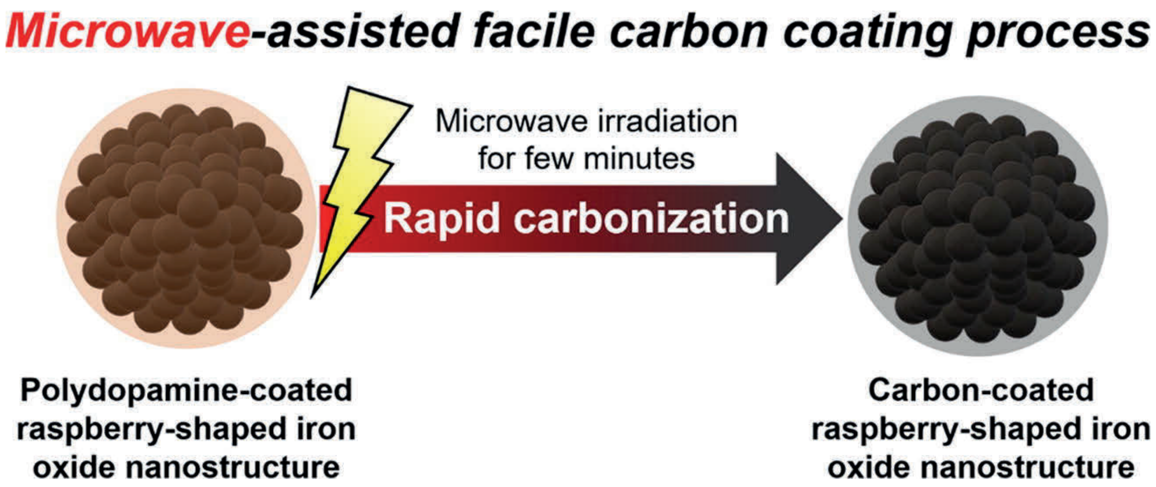
Poster Presentation : **ELEC.P-518**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Microwave irradiation-assisted facile preparation of carbon coating layer on raspberry-shaped iron oxide particles for lithium-ion battery anodes

Youngseul Cho, Yuanzhe Piao[1,*]

Graduate School of Convergence Science & Technology, Program in Nano Science & Technology, Korea
[1]*Graduate School of Convergence Science and Technology, Seoul National University, Korea*

Iron oxide/carbon nanocomposite has been receiving much attention as a promising anode material for lithium-ion batteries (LIBs) due to its high theoretical capacity, low cost, and environmental benignity. However, synthesizing nanostructured iron oxide/carbon composite typically requires complicated procedures with long-time pyrolysis of the carbon precursors at high temperatures. In order to address the challenges of conventional heat treatment, microwave-induced carbonization has been proposed as an effective method with its multiple advantages including synthetic simplicity, short processing time, and low energy consumption. Herein, we report a facile preparation of carbon coating on raspberry-shaped iron oxide nanostructure (RSIN) via microwave irradiation. In this work, the RSIN was synthesized via a one-pot polyol solvothermal method and the resulting RSIN shows a superparamagnetic property. The unique magnetic property of RSIN provides efficient microwave absorption, thus enabling rapid carbonization of polydopamine coating on its surface within a few minutes. The carbon-coated RSIN via microwave irradiation (MW-pRSIN) is electrochemically tested as anode material for LIBs. In terms of electrochemical performance, MW-pRSIN exhibits a high reversible capacity of 415 mAh g-1 in the first step at 8.0 A g-1 and good cycling performance (87.5 % capacity retention after 1000 cycles at 2.0 A g-1). Interestingly, the MW-pRSIN shows better electrochemical performance compared to that of conventional heat-treated one. This result is attributed to the efficient localized heating of microwave irradiation. The unique carbonization method using microwave could be helpful to design carbon-coated magnetic particles and promote scientific advances in many other fields.


Microwave-assisted facile carbon coating process
Microwave irradiation for few minutes
Rapid carbonization
Polydopamine-coated raspberry-shaped iron oxide nanostructure
Carbon-coated raspberry-shaped iron oxide nanostructure

Poster Presentation : **ELEC.P-519**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

[Withdrawal] Nb5+ Doped Core-shell Layerd High Nickel Cathodes For Rapid Charging And Dramatic Cycling Performance

Eui Jeong Park, Jong-Tae Son*

Department of Nano-Polymer Science & Engineering, Korea National University of Transportation, Korea

Poster Presentation : **ELEC.P-520**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Heteroatom Doped Carbon Supported Low Content of Pt as An Efficient Catalyst for Hydrogen Evolution Reaction in Both Acidic and Alkaline media

Yuan hui Huang, Kyeong-Deok Seo[1], Deog Su Park[2], Yoon Bo Shim[1,*]

Molecular Science Technology, Pusan National University, China

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

[2] *Pusan National University, Korea*

Tiny amount of Pt nanoparticles decorated N, P doped-carbon (Pt/NPC) was firstly prepared via simple microwave irradiation of resin sphere derived carbon followed by phosphorization step. The synergistic effects between embedded Pt nanoparticles and N, P doped carbon strongly promote the hydrogen evolution reaction (HER) performance, which exhibits mass activity 3.3 and 3.8-fold greater than that of commercial 20% Pt/C at an overpotential of 100 mV under acidic and alkaline media, respectively. The electronegativity differences between C, N and P dopants can modulate the electronic state density of carbon to produce new active sites for HER. Moreover, due to donation of charge from N and P to Pt, Pt nanoparticles can be uniformly dispersed on carbon network, affording an excellent stability compared to Pt/C during the long-term duration test. We expect that this heteroatom doping strategy opens a new avenue to design low content of Pt electrocatalyst along with excellent catalytic activity for HER.

Poster Presentation : **ELEC.P-521**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Development of H2O2 sensor using bimetals nanocatalysts

baby Nimisha, Kyeong-Deok Seo[1], Deog Su Park[2], Yoon Bo Shim[1,*]

Chemistry of material, Pusan National University, India
[1]*Department of Chemistry, Pusan National University, Korea*
[2]*Pusan National University, Korea*

Comparison of Au, Mn, Ni, Cu bimetals nanoparticle composited conductive polymer electrodes have been performed for the detection of hydrogen peroxide. The bimetal NPs were prepared by reducing metal chloride (Au, Mn Ni, Cu) in optimized conditions (concentration, molar ratio and reaction time). The proposed sensor was characterized employing cyclic voltammetry and electrochemical impedance spectroscopy to evaluate electrical and electrochemical properties of each modified layer. In addition, the surface analysis using XPS, EDS, and SEM were carried out to evaluate the chemical binding, composition and morphology. The composite electrode showed well-defined voltammetric peak for the oxidation of H2O2 at ~0.6 V and was able to detect H2O2 from 1.0 μM to 10 mM concentration with detection limit of 0.4 μM.

Poster Presentation : **ELEC.P-522**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Sandwich-like $Na_2Ti_6O_{13}$/rGO Composite as an Anode Material for High Performance Sodium-Ion Batteries

Jungwook Song, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Sodium-ion batteries (SIBs) have been attracted as large-scale energy storage systems (ESSs) due to low cost and abundant reserves of sodium resources compared to lithium. $Na_2Ti_6O_{13}$ is an attractive material as an anode in SIBs because of its tunnel structure that can provide long-term cycle stability due to high Na^+ diffusion and good ionic conductivity. However, the major issue is its low theoretical capacity of 49 mAh g^{-1}. In order to solve this issue, sandwich-like $Na_2Ti_6O_{13}$/rGO was prepared via the liquid-phase exfoliation and restacking through electrostatic interaction. With this unique morphology, it can provide many active sites associated with sodium storage. Sandwich-like $Na_2Ti_6O_{13}$/rGO composite showed an improved reversible capacity and cycle stability with an initial discharge capacity of about 385.3 mAh g^{-1} and 176.9 mAh g^{-1} after 500 cycles at 0.1 A g^{-1} and 0.01-2.5 V compared to bare $Na_2Ti_6O_{13}$.

Poster Presentation : **ELEC.P-523**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Enhanced Redox Reversibility of FeF_2 Coated by Electron-Rich N-Doped Graphitic Carbon as Cathode Material for Sodium-Ion Batteries

Achmad Yanuar Maulana, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Sodium-ion batteries (SIBs) have received increasing attention as a good prospect for future battery systems than lithium-ion batteries due to the high abundance and cheaper price of sodium. Currently, many studies of cathode materials in SIBs are dominated by insertion-type cathodes. However, the low theoretical capacity of insertion-type cathodes will be an obstacle to make the high energy density of SIBs. Iron difluoride (FeF_2) has been considered as a promising conversion-type cathode material in SIBs due to its low cost, high working potential, and theoretical capacity (571 mAh g^{-1}). However, the irreversible redox reactions of FeF_2 become the main issue in the SIBs system as reported in the previous reports. In this study, the redox reversibility of FeF_2 was successfully enhanced in SIBs by coating the FeF_2 particles with electron-rich N-doped graphitic carbon (FeF_2@NGC). The FeF_2@NGC showed an increase in reversible discharge capacity of about 233.2 mAh g^{-1} after 300 cycles at a current density of 50 mA g^{-1} compared to bare FeF_2 (24.2 mAh g^{-1}).

Poster Presentation : **ELEC.P-524**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

$Na_{0.8}Ti_4O_8$/C Composite Prepared with Resorcinol as an Anode Material for Sodium-Ion Batteries

Chaeeun Lee, Hyunjeong Gim, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Lithium-ion batteries (LIBs) are widely used in energy storage devices and their use is increasing continuously. However, the limited lithium reserves will drive up prices due to resource depletion in the future, making it hard to be used in large-scale energy storage devices. Therefore, sodium-ion batteries (SIBs) are attracted as an alternative substitution for LIBs because of the lower cost and larger abundance of Na. Many studies have reported that graphite as a commercial anode in LIBs is not suitable in the SIBs system due to the higher size of the Na^+ ion. Several sodium titanates (NTOs) series such as $Na_2Ti_3O_7$, $Na_2Ti_6O_{13}$, and $Na_4Ti_5O_{12}$ have been explored as anode materials in SIBs because of their excellent cycle stability, ion conductivity, and storage capacity. However, the $Na_{0.8}Ti_4O_8$ has rarely been studied due to the difficulty of synthesis caused by the unstable oxidation number of Titanium (3.8) compared to another NTOs materials (4). In this study, we synthesize the $Na_{0.8}Ti_4O_8$/C composite derived from resorcinol by adjusting the resorcinol contents. The $Na_{0.8}Ti_4O_8$/Cx0.5 sample exhibited an excellent reversible discharge capacity of about 189.8 mAh g^{-1} after 100 cycles at a rate of 0.1 A g^{-1} in the 0.01–2.5 V voltage range.

Poster Presentation : **ELEC.P-525**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

The Effect of Ni doping in FeOF as a Cathode Material for Enhanced Electrochemical Performances for Sodium-Ion Batteries

Da won Lee, Boram Yun, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

In the future, the implementation of lithium-ion batteries (LIBs) in large-scale energy storage systems will encounter some difficulties due to the low abundance and rising price of lithium. Sodium-ion batteries (SIBs) are promising as an alternative battery system because of the cheaper price of sodium and its higher resources. In addition, SIBs have similar energy storage mechanisms to those of the LIBs. Recently, research about cathode materials in SIBs was dominantly focused on intercalation-type cathodes such as $Na_3V_2(PO_4)_3$, $Na_3V_2O_2(PO_4)_2F$, and $Na_3V_2(PO_4)_2F_3$. However, their low theoretical capacitites have limited the energy density of SIBs. Iron oxyfluoride (FeOF) is a promising material for SIBs due to its low cost and higher theoretical capacity (~855 mAh g^{-1}). However, FeOF still exhibits poor cycling stability, rate capability, and low initial coulombic efficiency caused by its low electrical conductivity and slow ion diffusion. To solve these problems, we investigated the Ni doping effect to balance reversible high capability and structure stability of FeOF. The $Fe_{1-x}Ni_xOF$ (x = 0.007-0.3) electrodes represent good cyclic performance, for example, a reversible discharge capacity of 450.4 mAh g^{-1} with a fading rate of 0.21% per cycle after 100 cycles at 100 mAh g^{-1} in the voltage range of 1.2-4.0 V.

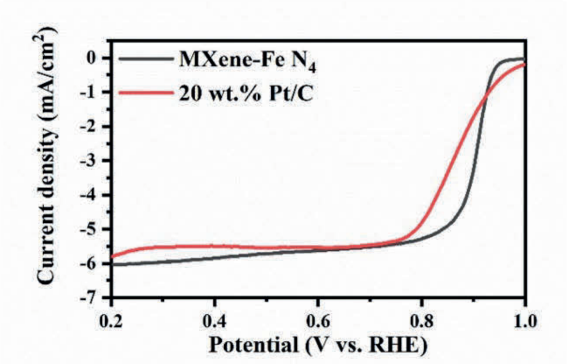
Poster Presentation : **ELEC.P-526**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Development of Single Atomic Fe-N4 anchored Ti3C2Tx MXene for Highly Superior ORR Electrocatalyst: Based on Plasma Induced strong Metal – Metal Interaction

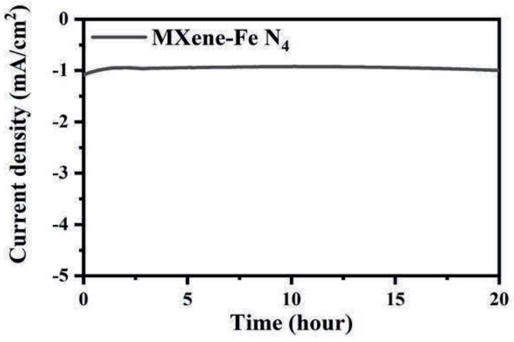
Seonghee Kim, Oi Lun Helena Li[*]

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

After global carbon neutral policies are actively ongoing, demand of environment friendly energy devices such as fuel cell and metal-air batteries is rapidly increasing. However, currently used electrocatalysts are using expensive platinum group metal (PGM) such as Platinum or Palladium. Among them, single atomic Fe metal, as the most promising candidate, showed extraordinary performance from the numeral experimental reports. However, low chemical tolerances of the single atomic Fe structure on the carbon substrate retarding its practical application to the industrial usage. To solve this major drawback of the carbon-based structure, several challenges are tried to develop stable substrate from non-carbon materials. Especially, recently reported Ti3C2Tx MXene 2D material takes notice as the promising substitute of the carbon substrate. But, due to the difficulty of the making strong bonding between single atomic Fe structure and metallic MXene substrate, it showed relatively low durability due to the weak interaction between atomic Fe and MXene substrate. So, here in, we report single atom Fe-N4 anchored MXene electrocatalyst induced from the novel plasma engineering process. In this research charged electrons activate the surface of the MXene during the plasma process, and Fe-N4 active ORR structure strongly anchored with the MXene substrate. As a result, plasma induced MXene-FeN4 electrocatalyst showed extremely high ORR activity of E1/2: 0.906 V vs. RHE which is ~50 mV positive performance compared to benchmark 20 wt.% Pt/C. Also, showing much more enhanced stability over 20 hours even far better than currently reported MXene based single atom Fe electrocatalyst.



ORR LSV curves of the synthesized MXene-FeN4 and Pt/C in 0.1 M KOH



CA profile of the synthesized MXene-FeN4 over 20 hours in 0.1 M KOH

Poster Presentation : **ELEC.P-527**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Al-doped Co9S8 encapsulated by nitrogen-graphene for solid-state asymmetric supercapacitors

Emad S. Goda, Sang Eun Hong[*], Kuk Ro Yoon[*]

Department of Chemistry, Hannam University, Korea

Herein, a novel type of core/sell architecture was successfully designed from aluminum-doped cobalt sulfide encapsulated by nitrogen-doped graphene (Al-doped Co9S8@NG) through the solvothermal/sulfuration of ZIF67 structure subsequent by wrapping with Ppy layer and calcination in argon gas at various temperatures. The developed core-shell material was utilized as a promising cathode material for solid-state asymmetrical supercapacitor device (AsScs). Interestingly, integrating the morphology, and composition merits could upgrade the Al-doped Co9S8@NG600 electrode with highly enhanced supercapacitive features. The electrode was attained a supreme capacitance of about 1472 F/g at an applied current density of 1 A/g, ultra-long cycle stability of 92% after performing 10000 cycles, and a remarkable retention rate (~71%). Motivally, Al-doped Co9S8@NG core/shell as a positive electrode was assembled with a negative electrode synthesized from activated PANI-derived carbon nanorods (ACNRs) in a solid-state AsSCs device. The device could give outstanding values from specific capacitance, energy density, and power density of 134 F/g, 41.9 Wh/kg, and 0.75 kW/kg, respectively with a considerable cycle life stability of 93% after consuming 10000 cycles. Further, when two AsSCs devices were linked in series, multicolor LED could be lightened for 25 s approving their availability for making modern portable electronics.

Poster Presentation : **ELEC.P-528**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

A hybrid CuO/N-CD/CNTs catalyst with high activity and durability for oxygen reduction reaction in alkaline solution

Jaemun Kim, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Electrocatalysis for the oxygen reduction reaction (ORR) play a significant role in electrochemical energy conversion and storage devices, such as fuel cells, batteries, and redox-flow batteries. In particular, traditional catalysts, such as Pt and its alloys, are commonly used as electrocatalyst materials for the ORR. However, Pt cannot be used in fuel cells or other energy system on a large scale because of expensive and limited resources. As an alternative, the design of highly active and stable catalysts using non-noble and carbon-based nanomaterials has focused attention more recently due to their relatively good ORR activity, stability, greater abundance and cost-competitive replacements compared to Pt. Herein, we report an efficient synthesis of hybrid copper oxide decorated carbon nanotubes with N-doped carbon dots (CuO/N-CD/CNTs) nanostructure in an aqueous solution and their electrocatalytic activity for ORR. Thermal pretreatment of CNT sheets plays a vital role in the structural CuO/N-CD/CNT formation. The composite has been evaluated using X-ray powder diffraction, scanning electron, and transmission electron microscopy. The catalytic activity for ORR was examined using cyclic voltammetry and linear-sweep voltammetry techniques. The CuO/N-CD/CNT catalyst exhibited excellent electrocatalytic activity in an alkaline solution compared to other composites (N-CD/CNTs and CuO/CNTs). This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614) and (No. 2021R1F1A1063825).

Poster Presentation : **ELEC.P-529**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

FeMo-MIL-88B nanorod derived 3D rod-shaped porous iron-molybdenum oxynitride for overall water splitting reaction

Tianyu Chen

Department of Applied Bioengineering, Graduate School of Convergence Science and Technology, Seoul National University, Korea

Due to excessive consumption of fossil fuels and relevant environmental pollution issues, much efforts have been made in the development of efficient and inexpensive electrocatalysts for sustainable and clean hydrogen energy generation. Herein, an ultrafast microwave-assisted synthesis of FeMo-MIL-88B followed by annealing at high temperature via soft-urea path is reported. The introduction of nitrogen element remarkably modifies the morphology and endows the material with large catalytic surface area. The transformed 3D rod-shaped porous iron-molybdenum oxynitride (FeMoON) presents outstanding electrocatalytic performances in hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and overall water splitting. The FeMoON electrode affords high current densities of 850 mA cm−1 at an over-potential of merely 364 mV for OER and 750 mA cm−1 at an overpotential of 400 mV for HER. The overall water-splitting demeanor surpasses that of commercial noble metal pair in high current densities and shows good stability during long-term uninterrupted testing. This work provides a promising way to design efficient and low-cost electrocatalyst for overall water splitting.

Poster Presentation : **ELEC.P-530**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Colorimetric and Electrochemical Detection of Glucose Using a Novel Fe-complexed Conducting Polymer

Golam Mahmudunnabi, Khatun A Jannath, Yoon Bo Shim[1,*]

Molecular Science Technology, Pusan National University, Korea
[1]*Department of Chemistry, Pusan National University, Korea*

We synthesized a novel Fe-Poly-DAN-TMB complex which has been used for ultra-sensitive detection of Glucose. Fe-Poly-DAN was synthesized using 1,8-Diaminonaphthalene as a monomer and $FeCl_3$ as a metal source and oxidizing agent. The morphology and the structure of the metal-polymer complex were confirmed by SEM, TEM, EDAX, and XPS. Glutaraldehyde has been used to crosslink between TMB and Fe-Poly-DAN. Fe-Poly-DAN showed superior peroxidase mimic activity though iron content was relatively less. To detect glucose, glucose oxidase mediated catalysis of glucose produces hydrogen peroxide which in turn is used by Fe-Poly-DAN in situ to change the colorless TMB to blue colored product, aids in naked-eye detection of glucose. Furthermore, for quantitative detection, we analyzed the reaction product in a simple gold nanoparticle modified electrode. As oxidized TMB is electroactive, it showed concentration dependency glucose used in the colorimetric reaction and analytical performances support that our method could be useful in clinical detection of glucose in Hyperglycemic and hypoglycemic patients.

Poster Presentation : **ELEC.P-531**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Entropymetry for detecting micro-cracks of high-nickel layered oxide cathodes

Minsoo Kim, Jang Wook Choi*

Seoul National University, Korea

With an explosive increase of electric vehicles (EVs), non-destructive monitoring of degradation in lithium ion batteries became more important for real-time diagnosis of EVs. As demand for increase of mileage, high-nickel cathodes have been adopted while high-nickel cathodes suffer from various degradation such as micro-cracks. Here, we introduce entropymetry for monitoring the structural change of NMC811 cathode along the state of charge (SOC) and structural degradation. Entropy change corresponded with structural change during charge, especially at the 4.2V region which occurs a sharp reduction of c-axis lattice. Entropy change at the 4.2V region decreased after degradation, which was attributed to heterogeneity of sites for lithium ions due to structural degradation from cation mixing and micro-cracks. In-situ XRD estimated structural heterogeneity through peak broadness at the 4.2V region. Structural degradation causes the reduction of equivalent energy states for Li ions and results in decrease of configurational entropy. Entropy change shows conditions of structural heterogeneity from different voltage cut-off and cycle number. The present study proposes entropymetry as the non-destructive tool for detecting micro-cracks of high-nickel layered oxide cathodes in lithium ion batteries.

Poster Presentation : **ELEC.P-532**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Nano/Microscale Integrated Mushroom-Shaped Hydrophilic CoP@Ni-CoP with Optimized Gas Bubble Release for High-Performance Water Splitting Catalysis

Xinyu Qin

Department of Transdisciplinary Studies, Seoul National University, Korea

Highly efficient electrocatalysts based on transition-metal phosphides (TMPs) for both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) via water splitting is receiving considerable attention in recent decades. Owing to the intrinsic sluggish kinetics, it is crucial to maximize reactivity to both HER and OER, especially in basic environment. This work describes the construction of cobalt phosphide@nickel-cobalt phosphide (denoted CPNCP) for overall water splitting in alkaline environment. Via a nanoscaled array type 'body' and microscaled 'head' structure, CPNCP presents high hydrophilicity and effective gas bubble release, contributing a prospective goal of efficient water splitting device for practical use. Remarkably, the fabricated CPNCP only needs a cell voltage of 1.49 V for driving overall water splitting to reach the current density at 10 mA·cm−2, and could run over 40 hours with little increase of applied voltage for continuous cycling at10 and 200 mA·cm-2. This work may shed some light on optimizing TMPs catalysts based on structure-activity relationship, and promote their applications in practical water splitting and other renewable energy options.

Poster Presentation : **ELEC.P-533**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Hierarchically constructed Hollow Ag-Au Nanospheres Covered with Pt Nanoclusters for Methanol Oxidation Reaction

Bingyi Yan

Department of Transdisciplinary Studies, Seoul National University, Korea

Based on galvanic replacement technology, a structurally innovated synthetic method of Pt nanocluster-anchored hollow Ag-Au nanostructures and measurements of their electrocatalytic properties for methanol oxidation reaction (MOR) are reported. The hollow interior of Pt nanocluster-anchored Ag-Au nanostructures and changes in the size of Pt nanoclusters by varying the injected molar ratio of Pt/Au were observed. Additionally, other morphological, compositional, and optical information of the obtained nanoscale materials were analyzed. The robust electrocatalytic ability of the obtained Pt nanocluster-anchored hollow Ag-Au nanostructures toward MOR was confirmed, which was endowed by largely exposed electrochemically catalytic surface area and appropriately scattered active sites. More importantly, the ease of the three-step synthetic strategy of the Pt nanocluster-anchored hollow Ag-Au nanostructures displayed their promising potential in the use of electrochemical oxidation of methanol. The synthetic strategy outlined here would open a new avenue for the engineering of noble-metal nanocrystals for a broad range of applications.

Poster Presentation : **ELEC.P-534**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Incorporation of Many Structural Features into a PtCo@Pt Nanowire as a Bifunctional and Durable Electrocatalyst for PEMFC and Water Electrolyzer

Gyan-Barimah Caleb, Jong-Sung Yu[1,*]

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

[1]*Department of Energy Science and Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

High performance and durable Pt-based electrocatalysts are necessary for the industrial application of fuels. Nanostructures such as metallenes and nanowires have gained significant attention in this field owing to their unique catalytic properties that can easily be manipulated to achieve desirable performance. Herein, we report a remarkable one-dimensional L1o ordered intermetallic PtCo alloy catalyst endowed with a compressively strained Pt-rich multi-faceted shell, prepared through a two-solvent system. The robust PtCo nanowires (NWs) exhibit excellent Pt utilization for oxygen reduction (ORR) displaying a half-cell mass activity of 1.30 A/mg_{Pt} with superior peak power performance in a single cell membrane electrode assembly (MEA) relative to the state-of-the-art commercial Pt/C. DFT calculations reveal that the high indexed Pt-(221) facet possesses the closest to optimum adsorption energy for oxygen species. Importantly, the L1o ordered intermetallic core, the thick Pt rich shell, and the one-dimensional anisotropy provided catalytic durability in both liquid half-cell and PEMFC single-cell durability tests. The catalyst also proved to be highly active and durable for hydrogen evolution reaction (HER) in both acidic and alkaline media.
Keywords: intermetallic, nanowire, PEMFC, ORR, HER, DFT

Poster Presentation : **ELEC.P-535**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Temperature Engineering of Copper Surface for Selective CO2 Electroreduction

Seongwoo Jo, Hyun Seo Ahn[1,*]

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

Electrochemical carbon dioxide reduction reaction(CO2RR) on copper has been emphasized for producing various hydrocarbons. But also it has suffered for its low selectivity. Most of studies are focusing on designing catalysts based on copper. Besides, the effect of electrolyte temperature on CO2RR has been shown to change reaction parameters and affect product distribution, suppressing Hydrogen evolving reaction(HER) and increasing amount of methane. In this study, We varied only temperature of the electrode surface and investigate the effect of local temperature near electrodes on CO2RR and adsorption/desorption chemistry of intermediate-metal surface. Along with pulse effect, more than 80% of methane was obtained from pristine copper foil electrode. The effect of local temperature and the mechanism of methane production in CO2RR are explained by using COMSOL Multiphysics simulation.

Poster Presentation : **ELEC.P-536**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Unraveling the source of irreversibility in Zn electro-deposition

Sunwoo Park, Jinho Chang*

Department of Chemistry, Hanyang University, Korea

Zn metal has been widely regarded as promising anode for aqueous battery because of low cost, safety and environmentally friendly. However, Zn anode have problems at low coulombic efficiency (CE) during Zn deposition/dissolution reaction due to side reactions in mild acidic electrolytes. it is necessary to unravel the source of irreversibility in order to provide the insight for solving the problem. We here report the electrochemical and spectroscopic analysis of zinc elecro-deposition/dissolution on Glassy carbon (GC) electrode in mild acidic condition with various anion. We found the difference with anion species in coulombic efficiency to Zn redox reaction. The coulombic efficiency of the Zinc deposition/dissolution reaction was high and stable in the solution containing chloride or acetate anion while relatively low in the sulfate anion. Then, we found the oxidative species in more positive potential than standard potential of Zn2+/Zn redox reaction through Cyclic voltammetry (CV) in sulfate electrolytes.

Poster Presentation : **ELEC.P-537**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Triiodide-in-iodine network: accelerant for iodide transport in quaternary ammonium iodide-iodine solution

Hyeonmin Kim, Jinho Chang[*]

Department of Chemistry, Hanyang University, Korea

Zn-polyiodide redox flow battery has been considered the promising energy storage systems. In its charging process, however, charge transfer kinetics of I$^-$-oxidation often suffers from intrinsically generated iodine film on a cathode of the battery. Therefore, it is crucial to understand reason for a slow kinetics of I$^-$-oxidation on the cathode modified with an iodine film, and to control physicochemical properties of the film.Here, as an effort to understand and modulate an iodine film, we introduce an electrochemically generated N-methyl-N-ethyl pyrrolidinium iodide-iodine solution, designated as MEPIS. We found charge transfer kinetics of I$^-$-oxidation is dramatically enhanced compared to an iodine film generated from a conventional electrolyte condition, which is revealed to be associated with stable formation of a triiodide-iodine ($I_3^-\cdot(I_2)_n$) network in MEPIS. Raman spectroscopic and electrochemical analyses showed that composition of electrochemically generated MEPIS was changed from I_3^- to $I_3^-\cdot(I_2)_n$ via I_5^- as anodic overpotential increased. We confirmed that I$^-$ is electrochemically oxidized on a Pt electrode modified with MEPIS without kinetic limitation. i.e. MEPIS can acts as a metallic electrode for electro-oxidation of I$^-$, which is contrary to the nature of an iodine film derived from a NaI solution as an activation barrier of I$^-$-oxidation. Through stochastic MEPIS-particle impact electrochemistry and electrochemical impedance spectroscopy, we revealed that the enhanced charge transfer kinetics for I$^-$-oxidation in MEPIS would be originated from an existence of freely moved I_3^- because of its weak interaction with I_2 in a $I_3^-\cdot(I_2)_n$ network.

Poster Presentation : **ELEC.P-538**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Charateristic of metal/electrolyte interface at water-in-salt electrolyte (WISE): chloride oxidation mechanism in WISE

Sungjun Son

Department of chemistry, Hanyang University, Korea

Recently, water-in-salt electrolyte (WISE) have been recognized with promising electrolyte instead of organic electrolytes in Li-ion battery because of improved safety and stability. Moreover WISE ,superconcentrated aqueous solution, offer wide electrochemical potential window. Therefore WISE is used in lots of electrochemical devices. However WISE is not well known that electrochemical mechanism of how it is structured metal/electrolyte interface and what kind of character. We investigated electrochemical behavior of chloride at WISE with concentration ranging from 3 to 21m lithium bis(trifluoromethylsulfonyl)imide (LiTFSI). As concentration of LiTFSI increase, chloride oxidation peak is not devided at platinum (Pt) electrode. In contrast to Pt, chloride oxidation peak is devided into two at gold (Au) and glassy carbon (GC) electrode. This provides that chloride is always oxidized to chlorine via trichloride and that the intermediate can be stabilzed on Au and GC electrode, but not on Pt electrode. Using that chloride is oxidized to chlorine in aqueous solution and trichloride is stabilized in IL or organic solvents, chloride oxidation show that there is film on surface which is similar to IL characteristic, because positively charged electrode is compensated by {rm TFSI}^- anion and anion is bulky and hydrophobic also water molecules are excluded from electrode.

Poster Presentation : **ELEC.P-539**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Flexible Li-ion battery via one-pot synthesis

Hun Seong Kim, Hyunyoung Jung[1,*], Senthil Chenrayan, SunSik Kim[2]

Energy Engineering, Gyeongsang National University, Korea
[1]Department of Energy Engineering, Gyeongsang National University, Korea
[2]Gyeongsang National University, Korea

Lithium-ion batteries are one of the most interesting fields in the world. Numerous efforts have been devoted to increasing the capacity, power density, and cycling performance. Transition metal oxide-based anodes are an attractive candidate for high performance Li-ion batteries due to their high theoretical capacity. However, their practical applications are limited due to the volume expansion occurring during the intercalation/desorption process of lithium and the inactive material of the electrode. Here, we report a manganese oxide nanowires via one-pot formation method. The Mno2 anode is completed simply by freeze-drying a controlled in-situ hydrogel thin film with no additional process, achieving flexible devices without binder. The porous electrode structure made through one-pot synthesis suppresses volume expansion and maximizes capacity by making lithium ions more accessible. As a result, the MnO2/graphene electrode showed a capacity of 525 mAh/g at 1.0A/g 400th cycles. This study shows the possibility of one-pot synthesis as a method of making conversion-type electrodes for realizing ultra-light and flexible batteries.

Poster Presentation : **ELEC.P-540**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Graphene based nano-architectured conversion type SnO2 anode for long-life Li-ion battery

SunSik Kim, Hyunyoung Jung*, Senthil Chenrayan

Energy Engineering, Gyeongsang National University, Korea

Conversion-type materials are regarded as one among the prime candidates for the anodes of lithium-ion battery owing to their high theoretical capacity. In particular, tin oxide (SnO2) exhibits a high theoretical capacity of 1494 mAh g-1 through conversion-type electrochemical reaction with Li-ions. Concerns with respect to huge irreversibility and volume expansion upon electrochemical cycling is detrimental to the battery. Here, we report the formation of nanosized SnO2 particles through a simple and facile room temperature synthesis to be utilized as anodes for Li-ion battery. The bonding arrangement Sn-O-C persistent in the as-fabricated material is tuned to obtain Sn-C bond that enables to achieve a stable and high device performance. The Sn-C bonded material tested as an anode delivered a high initial discharge capacity of 1227 mAh g-1 at a current rate of 0.1 C with almost negligible irreversible capacity losses thereafter. Moreover, a good rate capability and cycle stability was achieved by the SnO2 anodes.

Poster Presentation : **ELEC.P-541**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Polymeric binders for the post Li-ion battery era

Senthil Chenrayan, Hyunyoung Jung[1,*]

Energy Engineering, Gyeongsang National University, India
[1]*Department of Energy Engineering, Gyeongsang National University, Korea*

Binders as a passive component of the electrodes play a key role to realize safer and improved electrochemical performance. The choice of binders varied with the evolution of different cell chemistries. Typically, post Li-ion cell chemistry era prerequisite for additional functionalities to be available from the binders to circumvent multiple concerns that arises during the battery operation. In this aspect, we have investigated the binder's choice considering the organic and polar binders employed to fabricate sulfur cathodes for the Li-S cell. It was found that the adhesion and limited-mechanical properties could be fulfilled through a linear chain polymer, whereas in addition the control of volume expansion and polysulfide capture requires a multi-functional binder.

Poster Presentation : **ELEC.P-542**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Attachable micropseudocapacitors based on highly swollen laser-induced-graphene

Yeong a Lee, Kyuyeon Jang[1], Hana Yoon[2,*]

Graduate school of energy science and technology, Chungnam National University, Korea
[1]University of Science & Technology, Korea
[2]Separation and Conversion Materials Research, Korea Institute of Energy Research, Korea

The rapid growth of miniaturized wearable and portable electronics has increased the demand for power sources that are sufficiently compact and can be directly integrated with them. Microsupercapacitors (MSCs) are recognized as the potential power supply devices due to their high power density, long operating lifetime and excellent rate performance. In this regard, MSCs with unique in-plane, interdigitated electrode design provide flexibility and ease of integration with wearable and portable electronics. However, MSCs are still limited in terms of design flexibility, scalability, reusability, and compatibility with basic components of wearable devices, such as textile, paper and plastic, etc. In this study, we report a high-performance sticker-type flexible microsupercapacitor using highly swollen reduced-graphene-oxide electrodes fabricated by a femtosecond-pulse laser to promote full active-site and durability of the electrodes.

Poster Presentation : **ELEC.P-543**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Highly stable and active PtP_2-based electrocatalyst for oxygen reduction in high temperature polymer electrolyte membrane fuel cell

Jeong-Hoon Yu, Jong-Sung Yu*

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

Platinum (Pt) is known to be the best and most effective electrocatalyst for the oxygen reduction reaction (ORR). However, given its high surface energy, it tends to lose its excellent catalytic activity after an unacceptably short period of usage. The stability of Pt has always been a bottleneck in commercializing the polymer electrolyte membrane fuel cell (PEMFC) technology. In high temperature-polymer electrolyte membrane fuel cells (HT-PEMFC), the activity loss has been traced back to the chemisorption of phosphate anions, irreversibly poisoning the active sites. Herein, we present an alternative platinum phosphide-based (PtP_2/C) electrocatalyst for the application under high temperature conditions. The prepared PtP_2/C catalyst shows surprisingly excellent long-time stability and catalytic activity in phosphoric acid. The improved stability is shown to be the product of lower adsorption strength of PtP_2 compared to Pt and better oxidation resistance of the carbon support in the presence of PtP_2.

Poster Presentation : **ELEC.P-544**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

MoS2-graphene composite with mixed phase of MoS2 and their application for lithium ion battery

Kyuyeon Jang, Yeong A Lee[1], Hana Yoon[2,*]

Advanced Energy and System Engineering, University of Science & Technology, Korea
[1]Graduate School of energy science and technology, Chungnam National University, Korea
[2]Separation and Conversion Materials Research, Korea Institute of Energy Research, Korea

Graphite and graphene are known to be very good anode materials for lithium ion batteries due to their excellent stability, but have a low theoretical capacity of 372 mAh/g. Electric vehicles and various electronic devices require a battery with a higher capacity than the current capacity, and it is essential to develop an anode material with a higher capacity. Therefore, anode materials using Si are in the spotlight. Si has a higher capacity (~4200mAh/g) than graphite materials, but there is a problem of volume expansion when the cycle is performed. Transition metal dichalgogenides (TMD) materials are attracting a lot of attention because of their excellent stability, low cost and high storage capacity. The theoretical capacity of MoS2 is known to be 670 mAh/g, making it a promising material for a LIB anode material. It is known to have 1T and 2H structures. The 1T phase has excellent conductivity as a anode material. 1T phase can be produced when a single layer is made through exfoliation. However, due to its meta stable structure, it is easily converted to the 2H phase as a stable phase. In this study, a composite of MoS2 and graphene was prepared by a chemical exfoliation method, and through this, a stable and high-capacity anode material was realized using the high energy storage capacity of MoS2 and the stability of graphene. In addition, a mixed phase of 1T and 2H structures was generated through the post-treatment process, and it was confirmed that the 1T phase was stably present. Through this, the diffusion of Li+ was facilitated by securing wide interface spacing and high conductivity of the 1T structure, and as a result, superior conductivity and high capacity were stably maintained compared to the single-phase material of the 2H structure.

Poster Presentation : **ELEC.P-545**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

One-pot synthesis of Mo-based catalysts for electrochemical nitrogen reduction reaction

Jihyun Kim, Yun Hwi Seong, Jun Ho Shim[*]

Department of Chemistry, Daegu University, Korea

Ammonia (NH_3) plays an important role in supporting global population owing to its role as an essential precursor for fertilizer production. On the other hand, the reactions require high temperature (~ 500 ℃) and pressures (>200 atm) and the use of noble metal-based catalysts. Indeed, the process is energetically demanding and associated with low efficiencies. Among various technologies, electrochemical method allows the direct conversion of renewable electricity into chemical bonds. For example, nitrogen gas molecules could be converted into NH_3 through the $6e^-$ process. In this study, novel metal-free Mo-based catalysts (MoX, X = Ni, Fe, Co, Cu) were developed as a highly efficient alternative catalyst for nitrogen reduction reaction (NRR). A dual-layer electrode is prepared by spraying the catalysts on carbon cloth, serving as the working electrode for nitrogen reduction to ammonia in an H-type cell. Other electrocatalytic activities was investigated by conventional electrochemical techniques. The compositional/structural features are characterized by high-resolution transmission electron microscopy, scanning electron Microscope, X-ray photoelectron spectroscope, and X-ray diffraction. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614) and (No. 2021R1F1A1063825).

Poster Presentation : **ELEC.P-546**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Highly efficient and stable g C3N4 decorated Ta3N5 nanotube on n-Si substrate for solar water oxidation

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

Advanced Chemicals & Engineering, Chonnam National University, Bangladesh

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

Poster Presentation : **ELEC.P-547**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

A Spin-Equilibrium Fe Complex for Aqueous Redox Flow Batteries

Donghwi Ko, Hye Ryung Byon*

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

Redox flow batteries (RFBs) are considered as promising grid-scale electrochemical energy storage, caused by the ensured safety, low cost and maintenance, and decoupled energy and power density. While vanadium has been commercially utilized as the redox-active material in aqueous RFBs, more economical materials such as Fe-based complexes are necessary for future RFBs. Ferrocyanide is a representative Fe complex showing the exceptionally stable and reversible redox process. However, many others showed unstable nature with water and air, poor solubility, and low electrochemical stability. Thus, better molecular designs of Fe complexes are required for RFBs.In this study, we introduced spin-equilibrium hexadentate Schiff-base ligand to the central Fe ion and investigated electrochemical stability correlated with the spin state of Fe ion. The selection of chelate ligands was essential to avoid ligand dissociation and also harness the spin state of the Fe ion. In addition, the pH of the aqueous media was significant to stabilize the Fe complex during the electrochemical redox process. We found that our Fe complex had a low spin state and high stability in the basic condition in contrast with poor stability in the acidic condition. The presentation will show stable RFB performances with our Fe complex as the negolyte (negative electrolyte) paired with iodide/triiodide as the posolyte (positive electrolyte) in mild alkaline solution.

Poster Presentation : **ELEC.P-548**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Electrodeposited Copper for Electrochemical Nitrate Reduction Reaction

Shim Minyoung, Hye Ryung Byon[1,*]

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

Ammonia has been widely produced through the Habor-Bosch process using N2 gas. However, because this well-known chemical process evolves CO2 byproducts and requires high temperature and pressure, the alternative electrochemical conversion process has been suggested. Here, we studied nitrate (NO3-) reduction reaction using the Cu catalyst to generate ammonia. The NO3- reactant is electrochemically more active than N2, and its conversion through the electrochemical reaction is beneficial as an aspect of environmental protection. We used electrodeposited Cu forming nano dendrite as the catalyst of the nitrate reduction reaction. Dendritic shape and high surface area of 3-D structured Cu showed lower overpotential and higher ammonia yield than flat Cu foil. In addition, we found that the rate-determining step was the conversion of nitrate to nitrite. It presumably arises from the difficulty of nitrate access to the Cu surface. To mitigate this problem, we designed to use highly charged cations that can pair with nitrate and approach the Cu surface together. In the presentation, I will discuss the role of Cu morphology and cation to improve the conversion efficiency of nitrate.

Poster Presentation : **ELEC.P-549**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

The effect of a high binding affinity with oxygen on anion redox reactions in Li-rich layered oxides

<u>Seung Gu Kim</u>, Hye Ryung Byon[*]

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

Recently, Li- and Mn-rich cathodes have been developed to improve capacity in Li-ion batteries. An excess of Li+ alters the oxygen molecular orbitals in the cathodes, resulting in the participation of oxygen-anion redox during the charging and discharging process. While employing both cation (i.e., transition metal) and anion redox reactions contribute to a capacity rise, the result of latter reaction such as diffusion of the oxygen atom and gas evolution of oxygen molecules impart to deform the cathode structure and rapid capacity fading. To mitigate these issues, we attempted surface doping of the Li-rich electrode, Li1.15Ni0.17Co0.17Mn0.51O2, using Zr4+, Sn4+, and Ru4+. These dopants have a high binding affinity with oxygen, thereby being expected to suppress oxygen evolution. We developed the synthetic method to introduce the dopants uniformly and observed that Sn-doped electrodes had better capacity retention after 200 cycles. I will discuss the role of dopants and related analyses details in the presentation.

Poster Presentation : **ELEC.P-550**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Electrochemistry in CO2-containing lithium-oxygen cells

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*

The lithium-air battery is one of the promising next-generation energy storages offering higher theoretical energy density than the current technology of Li-ion batteries. So far, lithium-“oxygen” cells have been intensively studied to understand essential oxygen chemistry. However, because the CO2 and H2O in the air significantly alter the overall cell chemistry, it is necessary to explore their roles and find the solution to improve cycling performance. We particularly focused on the CO2 gas having an impurity level (approximate 400 ppm) in the air while incredibly influencing oxygen chemistry. By using 10 v/v% of CO2 gas with 90 v/v% O2 gas, the CO2-containing lithium-oxygen cells produced predominant lithium carbonate (Li2CO3) during the discharging process instead of the expected primary product lithium peroxide (Li2O2). Along with Li2CO3, there were intermediate species and/or byproducts. We found that these intermediate/byproduct species seemingly offered lower overpotential for oxidative decomposition compared to that of Li2CO3 during the charging process. Therefore, it is essential to understand the redox process of these intermediate species in the lithium-oxygen cells and to find the optimum condition retaining these species prolong. This presentation will show analyses of these intermediate species using spectroscopy tools and online electrochemical mass spectrometry and their effects on cell performances.

Poster Presentation : **ELEC.P-551**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Effect of precursor on the formation of Ni-rich NCM material in lithium ion batteries

Park Seonhye, Cheolho Jeon*

Research Center for Materials Analysis, Korea Basic Science Institute, Korea

Ni-rich layered oxides are one of the promising lithium-ion battery materials due to their high energy density, high capacity and low cost. Especially, Ni0.92Co0.035Mn0.045O2 (NCM) cathode materials are synthesized as homogeneous spherical particles by co-precipitation. Various co-precipitation conditions such as stirring rate (RPM), NH3 concentration, temperature, and pH are key parameters to control the crystal structure and morphology of precursors. Herein, we studied the changes of surface morphology with controlling the synthetic condition. The thickness of NCM precursors was strongly affected by pH and NH3 concentration. The specific capacity of Ni-rich(>98%) NCM cathode with the synthesized at pH12.1 and 2 M NH3 particles is up to 258 mAh/g at 0.1 C.

Poster Presentation : **ELEC.P-552**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Influence of Conductive Carbon Additives in Lithium Organic Batteries

Joonhee Moon*, Munhwa Ryu[1]

Advanced Nano-Surface Research Group, Korea Basic Science Institute, Korea
[1]소재연구부, Korea Basic Science Institute, Korea

Organic electrodes of p-type are emerging cathode materials in rechargeable lithium ion batteries due to their high theoretical capacity, abundance of the elements, and structural tunability. However, organic materials show poor electrochemical performance due to their low electrical conductivity and low energy density. To solve these problems, we studied the effects of two types of carbon conductive additives, Ketjen Black and Super-P, in single organic molecule (dimethylphenazine, DMPZ) based lithium batteries. The different physical properties of the materials triggered different interactions between the various components. The changes of the surface structure were studied using Raman spectroscopy.

Poster Presentation : **ELEC.P-553**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Synthesis of new electron transfer mediators and polymer backbone for application to glucose sensing system

Hoejun Kwon, TaeHoon Kim[1], Bongjin Moon[1,*]

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

We synthesized various osmium metal compounds based on tris-2-pyridylmethylamine (TPMA) that can be applied as an electron transfer mediator in an electrochemical glucose sensor. In our study, we found that the osmium complex with multidentate TPMA is more stable than the one derived from mono or bidentate ligand. For the best performance of the glucose sensor, it is desirable for the electron transport mediator to have an oxidation/reduction potential in the range of -0.2 ~ 0 V (vs Ag/AgCl). We synthesized TPMA-based osmium complexes and investigated their electrochemical properties by cyclic voltammetry.In addition, the osmium complex and glucose dehydrogenase (GDH) for sensor application were fixed using a pentafluorophenyl acrylate (PFPA)-based polymer matrix, which is an activated ester that can be easily substituted with amines. The reaction progress between the PFPA polymer and the osmium complex having an amine group was confirmed using 19F NMR. The extent of the coupling reaction could be determined indirectly. From the electrochemical experiments using the electrode made with these materials, it was confirmed that the amount of current increased as the glucose concentration increases. The maximum current in the high concentration section was also determined.

Poster Presentation : **ELEC.P-554**
Electrochemistry
Exhibition Hall 1 THU 11:00~12:30

Copper Oxide Catalyst used for Electrochemical CO2 Reduction Reaction

Rohini Kanase, Soon Hyung Kang[1,*]

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

In recent years, Selective conversion of CO2 to fuels and chemicals has been deliberated one of the key challenges in the electrochemical CO2 reduction reaction (CO2RR). Copper (Cu)-based materials have been demonstrated for electro reduction of these products has received significant attention. In this work, we present development of Cu-electrocatalyst modified with copper aluminum (Cu80Al20) alloy on carbon paper (GDL). Firstly, we synthesis Copper aluminium alloy with different ratio by thermal evaporation method, second step to etched Al content in NaOH and formation of copper. Copper oxide (Cu2O) phase nanowire has formed on the carbon paper which confirmed by the XRD and XPS. These 2D nanostructured of Copper oxide nanowires confirmed by FE-SEM. Furthermore, electrochemical properties for CO2 reduction reaction performed in 1M aqueous KHCO3 electrolyte which shows high current density with less negative potential. Also, we obtain selective reduction of C2+ product such as Ethylene, Ethanol and Propanol up to 72% at -0.85VRHE and current density is -300mA/cm2. Etched copper aluminium shows selectivity and activity for C2+ product at low negative potential has confirmed

128th General Meeting of the Korean Chemical Society
October 13(Wed)~15(Fri), 2021, BEXCO, Busan, Korea

Poster Presentation : **ELEC.P-555**

Electrochemistry

Exhibition Hall 1 THU 11:00~12:30

Systematic and feasible surface engineering promotes significant photostability to GaN photoanode for solar water splitting reactions

Maheswari Arunachalam, Soon Hyung Kang[1,*]

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

- Withdrawal -

Poster Presentation : **EDU.P-556**

Chemistry Education

Exhibition Hall 1 THU 11:00~12:30

Development and effectiveness of education program to improve meta-modeling knowledge level for chemistry teachers

Yunji Nam, Seounghey Paik*

Department of Chemical Education, Korea National University of Education, Korea

- Withdrawal -

Poster Presentation : **EDU.P-557**
Chemistry Education
Exhibition Hall 1 THU 11:00~12:30

Analysis of the Inscriptions in the Basic Subject Textbooks for the Chemical Engineering Course in Specialized High School

Jin-Ju Rho*, **JaeYoung Han**[1]

Chungbuk Natioanl University, Korea
[1]*Department of Chemistry Education, Chungbuk Natioanl University, Korea*

In this study, we analyzed the inscriptions used in the textbooks for the chemical industry course. The textbooks analyzed were from the subjects of ‘industrial chemistry’, ‘manufacturing chemistry’, and ‘unit operation’, which are the basic subjects taught to students majoring in the chemical industry at the specialized high schools. The textbooks were selected in the 7th national curriculum, in the curriculum revised in 2009, and in the curriculum revised in 2015.As a result, in all three subjects, the number of inscriptions per page was the highest in the curriculum revised in 2015, which can be interpreted as the importance of using inscriptions in textbooks has grown. In addition, in the ratio of use of inscriptions by type, equation was overwhelmingly, and in the ratio of use of inscriptions by function, complementary functions were the most. These result can be interpreted as such inscriptions show the characteristics of the chemical industry specialty. There are a lot of equations in the unit operation textbook. The inscriptions of complementary functions can deliver many functions and technologies in the limited space of textbook and in the limited time of classes.Since students majoring in chemical industry have to learn professional and skilled practical skills, there are many parts that are difficult to understand with only linguistic information in classes through textbooks. Therefore, by recognizing the importance of inscriptions in textbooks in specialized high schools, it is necessary to conduct continuously the research related to the inscriptions in specialized subjects as well as in the basic subjects.

Poster Presentation : **EDU.P-558**
Chemistry Education
Exhibition Hall 1 THU 11:00~12:30

The effects of semantic mapping strategy on the inferential comprehension of high school students in reading scientific texts

Su-Jin Lee, 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 effects of implementing semantic mapping reading strategy in chemistry class on students' inferential comprehension and reading ability. The semantic mapping reading strategy was introduced to help students build better reading skills in science educational field. 3rd grade students of science core high school in a small and medium-sized city participated in this study for a semester. Texts with social science issues and chemistry subjects were used to implement semantic mapping reading strategy in the chemistry class. To investigate the changes in students' inferential comprehension and reading ability, experimental group students participated in the pre-reading and post-reading ability tests and the results were analyzed. And student's survey was also conducted to examine the usefulness of semantic reading strategy in reading science texts.

Poster Presentation : **EDU.P-559**
Chemistry Education
Exhibition Hall 1 THU 11:00~12:30

The Effects of Collaborative Problem-solving for Character Competence (CoProC) instruction model on character competence of elementary school students

Jaekyoung Jun, Jihun Park, Jiaeng Park, Geonu Kim, Jeonghee Nam[1,*]

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

The purpose of this study was to investigate an impact of the Collaborative Problem-solving for Character Competence (CoProc) instruction model to elementary school science classes. The Collaborative Problem-solving for Character Competence (CoProc) instruction model was developed to foster character competence within the context of secondary science education. In order to apply the CoProC program for elementary school students, five CoProC activities were developed that can be implemented within the context of elementary science education. Twenty-four fifth grade students participated in this study. The Character Competence Test was administered before and after and students' reflective writings. Students' character competence test result were collected and analyzed. After the intervention, questionnaires were also examined and analyzed. The result of this study shows a increase in the experimental group's character competence. Based on these result, we have found that CoProC instruction model would be an effective teaching intervention toward cultivating character competence in an elementary science education setting.

Poster Presentation : **EDU.P-560**
Chemistry Education
Exhibition Hall 1 THU 11:00~12:30

The Analysis of Character Competency Change in Elementary School Students through Collaborative Problem-solving for Character Competence (CoProc) instruction model

Jiaeng Park, Jeonghee Nam[1,*]

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

This study analyzed the effects of Collaborative Problem solving for Competency(CoProC) Instruction Model on the Character Compentence of elementary school students. In order to do so, for two classes of 32 students in fifth grade, Collaborative Problem solving for Competency(CoProC) Instruction Model had been applied to 5 topics for one class of experimental group consisting of 16 students, while experiment-oriented science classes which are commonly conducted in elementary schools were suggested to the other class of comparison group consisting of 16 students. In order to investigate the effects of the application of Collaborative Problem solving for Competency(CoProC) Instruction Model on the Character Competence of students, Character Competence test had been conducted on all the students in experimental and comparison group, after which it was analyzed. Then, the students in experimental group answered surveys after the classes. The findings were used to examine how Collaborative Problem solving for Competency(CoProC) impacts Character Competence of elementary school students. As a result of the study, in the total score of the Character Competence test, the experimental group students showed a statistically significant difference compared to the comparison group students in 9 sub-factors of Character Competence. Among them, responsibility showed the largest effect size, followed by honesty, self-regulation, collaboration, sincerity, tolerance, and empathy, and openness and consideration were average. Through the survey, the students recognized that the responsibility factor had changed the most among the nine Character Competence factors, which was consistent with the Character Competence test results. The results suggest that the Collaborative Problem solving for Competency(CoProC) Instruction Model to be an effective toward cultivating Character Competence of elementary school students.

Poster Presentation : **EDU.P-561**
Chemistry Education
Exhibition Hall 1 THU 11:00~12:30

Development of STEAM program for pre-service teachers based on analytical chemistry module-Observation of fine dust concentration in Jinju city using a portable fine dust meter (IV)-

Young Tae Kong

Science Education, Chinju National University of Education, Korea

In this study, the concentration of fine dust, which is one of the recent social issues, was measured using a portable fine dust meter, and based on the measurement activity and interpretation process, a STEAM program for elementary school teachers was developed.The portable fine dust detectors used in this study were Dylos 1700 (measurement interval of 1 minute) and Airguard K (Wi-Fi type, measurement interval of 5 minute). The measurement location was on the first floor of Chinju National University of Education, and measurements were made continuously for one month in March 2021. And in order to secure the reliability of the data obtained in this study, we compared it with the fine dust data obtained from the national monitoring stations installed in Jinju city.From the measurement results, the possibility of measuring the concentration of fine dust using a portable fine dust meter was confirmed. Also, changes in fine dust caused by yellow dust could be observed.The STEAM program for elementary school pre-service teachers was developed with the following focus on.S (Science,understanding of fine dust, etc.)T (Technology, fine dust measurement principle and understanding of national observatories, etc.)E (Engineering understanding of fine dust measuring equipment, etc.)A (Humanities and society, understanding regional changes in fine dust concentration, etc.)M (Mathematics, processing and graphing data obtained from national monitoring stations and measurements, etc.).[1] Home page of Korea Meteorological Administration and AirKorea, fine dust data [Public Information Data].This research was partially supported by the National Research Foundation of Korea (2016R1D1A1B02008712).

Poster Presentation : **EDU.P-562**
Chemistry Education
Exhibition Hall 1 THU 11:00~12:30

On the characteristics of the new high school chemistry curriculum in Japan (I)

Young Tae Kong

Science Education, Chinju National University of Education, Korea

In Japan, the elementary and junior high school science curriculum was completely revised in 2017, and the high school science curriculum was revised in 2018. According to this revision, a new high school chemistry textbook has been compiled and will be applied to high schools from April 2022.In this study, the characteristics of the new revision of the chemistry curriculum in Japan and the characteristics of the newly compiled high school chemistry textbooks were examined.First, the new chemistry curriculum in Japan emphasizes the 'cultivation of competencies' and emphasizes the cultivation of scientific inquiry (problem-solving learning) through observation and experiment. It also emphasizes ‘proactive, interactive and authentic learning’. Although there is no significant change compared to the previous curriculum in terms of learning content, polymer compounds were newly added to the properties of organic compounds in the 'Chemistry' subject. In addition, ‘The world pioneered by chemistry’ was added at the end of the ‘Basic Chemistry’ course to relate what is learned in chemistry to everyday life, and ‘The role of chemistry’ was added at the end of the ‘Chemistry’ course.The 'Basic Chemistry' textbook was compiled based on the content presented in the curriculum, such as proactive, interactive and authentic learning, an emphasis on the inquiry process, and an emphasis on systematicity in elementary, middle, and high schools. And, as the final chapter, ‘The world pioneered by chemistry’ was newly established.[1] MEXT (2018). National high school science curriculum, MEXT : Tokyo. This research was partially supported by the National Research Foundation of Korea (2016R1D1A1B02008712).

Poster Presentation : **EDU.P-563**

Chemistry Education

Exhibition Hall 1 THU 11:00~12:30

The Effect and Disturbance Factors of Practical-Based Teacher Education Program for the Development of TPACK in Pre-service Chemistry Teachers

Misun Jung, Seounghey Paik[1],*

Korea National University of Education, Korea

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

- Withdrawal -

Poster Presentation : **ENVR.P-564**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

[Withdrawal] Photoelectrochemical Activation of Reactive Bromine Species for Conversion of Ammonium to Dinitrogen

Seungmok Han, Wonyong Choi[*]

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

Poster Presentation : **ENVR.P-565**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

The Synthesis of Non-PFOA Typed Surfactant and Evaluation for Their Physical/Chemical Properties

Soo Youl Park

C1 Gas & Carbon Convergent Research Center, Korea Research Institute of Chemical Technology, Korea

Fluorinated surfactants, especially perfluorooctanoic acid (PFOA, C7F15COOH) derivatives with long fluorocarbon chain, are an aqueous anionic surfactants. However, they are harmful to human health and organic pollutant. In our aim, potential alternatives with shorter fluorocarbon chains have been synthesized. We investigated our surfactants with a sulfate anion group, hydrophobic chains, a hydrocarbon tail and a fluorocarbon chain or two fluorocarbon. We also were characterized their physical/chemical properties and It was found that these novel anionic surfactants have superior surface activities compared to PFOA derivatives.

Poster Presentation : **ENVR.P-566**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Solid-Solvent Hybrid Additive for Control of Morphology in Organic Solar Cells

Daehwan Lee, 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*

Most of the organic solar cells based on bulk-heterojunction type active layer are fabricated with the assistance of high-boiling-point solvent additives to optimize the phase separation of the donor and acceptor. The macroscopic phase separation can be controllable with this solvent additive. However, the control of the microscopic morphology (e.g. π-π stacking, orientation, etc.) inside phase is still dependent on the interaction energy and self-assembly characteristics of each donor and acceptor. In this work, we have introduced solid-solvent hybrid additive method on inverted PM6:Y6 solar cells to optimize both macroscopic donor-acceptor phase separation and the microscopic morphology at the same time. For the solvent additive, well-known 1-CN solvent additive was used to optimize macroscopic donor-acceptor phase separation. For the solid additive, newly synthesized 3D star-shaped solid additives (Star-A and Star-F), which were delicately designed to achieve adequate electrical property, electrostatic potential and geometrical structure was used to further optimize microscopic morphology. Grazing-incidence small-angle X-ray scattering (GISAXS) and grazing-incidence wide-angle X-ray scattering (GIWAXS) measurements showed that the star additives not only induce the dense and enhanced microscopic intermolecular π-π stacking within the phase, but also further optimize the phase separation. With hybrid additive method, further enhanced inverted PM6:Y6 solar cells was achieved with only 1% addition of star-series solid additives.

Poster Presentation : **ENVR.P-567**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Thermally Stable and Efficient Planar Perovskite Solar Cells by Introducing Novel IDTT-Based Small Molecule Additive

Hyuntae Choi, Seyeong Lim, Taiho Park[1,*]

Chemical engineering, Pohang University of Science and Technology, Korea

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

Perovskite solar cells (PSCs) have attracted attention for next-generation solar cells owing to their fascinating optoelectronic properties and solution processability. However, defects in PSCs, which adversely affect efficiency and stability, still remain an obstacle to commercialization. Herein, we developed a novel small molecule (SM) additive, indacenodithieno[3,2-b]thiophene (IDTT-THCz). The IDTT-ThCz is introduced to the perovskite layer and substantially passivates perovskite defects. Furthermore, this facile surface passivation also facilitates charge extraction and prevents perovskite degradation. The IDTT-THCz treated PSCs achieve a power conversion efficiency of 22.5% and retains 95% of their original efficiency under thermal stress.

Poster Presentation : **ENVR.P-568**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Highly Stable and Efficient CsPbI3 Perovskite Quantum Dot Solar Cells with Chloride-Passivated SnO2 Quantum Dots ETL

Sunhee Yun, Wooteak Jung[1], Taiho Park[2,*]

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

CsPbI3 perovskite quantum dots (CsPbI3-PQDs) with advantages of both perovskites and QDs have been studied as photoactive materials, surpassing a power conversion efficiency(PCE) of CsPbI3 PQDs solar to 15%. However, cubic-phase CsPbI3-PQDs show delta phase transition in ambient conditions, which ultimately reduces device stability. In this study, we introduced chloride-passivated SnO2 QDs (Cl@SnO2 QDs) as an electron transport layer (ETL). Cl@SnO2 QDs show higher photostability and lower surface defect compared to TiO2 nanoparticles, improving device operational stability significantly. Furthermore, the Cl@SnO2-based devices with enhanced open circuit voltage and current density showed PCE up to 14.5% compared to that of TiO2-based control devices (13.8%).

Poster Presentation : **ENVR.P-569**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Highly efficient perovskite solar cells with green-solvent processable, dopant-free and lead-capturable hole transport polymers

Wooteak Jung, Kyoungwon Choi, Hae Un Kim, Taiho Park*

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

With the recent developments in the efficient of perovskite solar cells (PSC), many different types of hole-transport layer (HTL) were synthesized with different functions. However, in PSC, environmental issue which results from the lead leakage problem could cause serious ecological system destruction. Here, we synthesized a novel donor-acceptor type polymer, alkoxy-PTEG, composed of benzo[1,2-b:4,5:b′]dithiophene and tetraethylene glycol (TEG)-substituted 2,1,3-benzothiadiazole, for highly efficient perovskite solar cells with lead-capturable hole transport property. Nuclear magnetic resonance revealed that TEG groups can efficiently chelate lead ion with moderate binding constant ($K_{binding}$ = 2.76) which resulted from PSC leakage. Furthermore, the alkoxy-PTEG showed high solubility not only in the commercial aromatic and halogenated solvents but also in nonaromatic solvents such as 3-methylcyclohexanaone (3-MC). Finally, a dopant-free alkoxy-PTEG device processed with 2-mehtyl anisole, which is a widely used food additive in industry, exhibited 21.2% efficiency in a tin oxide planar structure and showed 88% stability after 30 days ambient conditions. This is the first report to consider lead leakage and toxic processing solvents issue in the PSC.

Poster Presentation : **ENVR.P-570**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Reduction in Polydispersity of Perovskite Quantum Dots Enables Highly Efficient Solar Cells

Seyeong Lim, Daehwan Lee, Taiho Park*

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

Bandtail broadening, arising from increases in polydispersity of colloidal quantum dots (CQDs), results in deficits of open-circuit voltage (VOC) and deterioration of carrier transport in photovoltaics. For perovskite QDs (PQDs), which have attracted attention as a promising absorber material, the bandtail broadening due to their increased polydispersity during the polar solvent based purification process also limits the photovoltaic performance. Here, we demonstrate for the first time that the device performance of all-inorganic CsPbI3 PQD solar cells can be improved by using size-selected monodisperse PQDs. To effectively reduce the polydispersity in polar solvent purified PQDs, we employed size-selection of PQDs on the basis of gel permeation chromatography. Well-purified monodisperse PQDs obtained by this process show higher photoluminescence (PL) quantum yield, narrower PL full-width at half maximum (FWHM) and lower Urbach energy, in comparison with irregular-sized conventional PQDs. Therefore, CsPbI3 PQD solar cells using monodisperse Pe-CQDs show enhanced VOC (1.27 V) and power conversion efficiency (PCE) up to 15.3%, which is considerably higher than that of control devices using irregular-sized PQDs (1.22 V and 14.0% PCE).

Poster Presentation : **ENVR.P-571**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

High conductive crusty composite of Cu@NiCo/C for anode catalyst of alkaline fuel cell

Jihyeon Park, Jaeyoung Lee[1,*]

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

Although the use of non-platinum group metal (non-PGM) catalysts is the best way to reduce the price of fuel cells, it is hard to reach power performance of hydrogen-air fuel cells 1.0 – 1.2 W cm^{-2} in practical level. Hydrazine fuel cell which is one of the alkaline liquid fuel cells has been attractive for a long time due to its high energy density and a high theoretical potential without carbon emissions. In this study, we prepared a crust-like Cu@NiCo/C composite for an anode catalyst of direct liquid hydrazine fuel cell. The catalyst is synthesized through the facile polyol reduction process in which NiCo solution injected into Cu solution. To find a proper ratio, we systematically investigated their electro-catalytic performance of hydrazine oxidation and selected the optimized ratio of Cu@NiCo carefully. Through direct and indirect resistance measurements, we confirmed that introduction of copper could increase conductivity of the catalyst and enhance the adsorption of water. Consequently, as-prepared Co@NiCo/C showed a remarkable power density of 1.08 W cm^{-2} in the hydrazine fuel cell. The structure of catalyst keep its shape after more than eight times harsh cell test. We hope this strategy could expand the region of alkaline liquid fuel cell using non-PGM catalysts.

Poster Presentation : **ENVR.P-572**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Photoelectrochemical CO_2 Reduction into Liquid Solar Fuels on Cu-Sn Alloy with Reduced Graphene Oxide, Poly(4-vinylpyridine), and Nafion Layers as Cathode and BiVO4 as Photoanode

Stephanie restu Pratiwi, Ignasia Handipta Mahardika*, Hieu Minh Ngo*, Young soo Kang[1],*

Chemistry, Sogang University, Korea

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

Conversion of CO_2 into renewable energy sources has attracted extensive attention, not only decreases the CO_2 concentration in the atmosphere but also stores renewable energy. Photoelectrochemical (PEC) CO_2 reduction reaction (CO_2RR) has been studied by using several hybrid composite cathodes based on Cu-Sn alloy with $BiVO_4$ photoanode. Cu-Sn nanoparticles were prepared by phase and structure engineering to get core-shell structure as cathode whereas (040)-crystal facet engineered $BiVO_4$ was used as photoanode. Moreover, reduced graphene oxide (rGO) was coated on the surface of Cu-Sn layer to have sequential multi-electron shuttling process. Poly(4-vinylpyridine) (PVP) was coated on the surface of rGO/Cu-Sn layer to do CO_2 adsorption and activation to decrease activation energy of rate determining first electron transfer and reduction reaction energy for CO_2RR. PVP layer has been used as a catalyst to reduce the activation energy of the CO_2RR. Nafion (Naf) as proton-conductive polymer was coated on the surface of PVP/rGO/Cu-Sn layer to make one pot reaction of proton-coupled sequential multi-electron transfer from rGO to CO_2 reduction site. Naf is very well known as extremely high proton conductivity up to 10 mS/cm and negligible electron conductivity. This work suggests the new creative strategy to fabricate multi-functional hybrid composite electrode with high faradaic efficiency, solar-to-fuel performance, and high selectivity of CO_2RR to produce liquid product.

Poster Presentation : **ENVR.P-573**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Activation and Reduction of CO_2 for Solar Fuel Generation in Photoelectrochemical System with Hybrid Composite Ni_xFe_y Alloy and $BiVO_4$ Photoanode

Ignasia Handipta Mahardika, Stephanie Restu Pratiwi[1,*], Young soo Kang[2,*]

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

Due to its excellent electrochemical catalytic properties such as large charge capacity and high current density, nickel-iron (Ni_xFe_y) alloy can be a potential candidate of photoelectrochemical (PEC) catalyst of cathode for the CO_2 reduction reaction. Combination of (040)-$BiVO_4$ crystal facet engineered photoanode and (Ni_xFe_y) alloy hybrid composite cathode will create a successful PEC system due to its improvement of charge carrier mobility and high photocatalytic active sites for solar light energy conversion PEC CO_2 reduction is a promising method for artificial photosynthesis after the first report on photocatalytic water oxidation reaction with TiO_2 by Fujishima and Honda in 1972. Ni_xFe_y alloy as the pristine base catalyst of hybrid composite cathode material which was further developed as Ni_xFe_y/rGO/PVP/Nafion for the CO_2 activation, sequential multi-electron shuttling function and reduction potential tuning for the product selectivity. The coating of reduced graphene oxide (rGO) and poly(4-vinylpyridine) (PVP) layer on the cathode surface with homogeneous and even thin thickness can have each function to increase charge capacity and to activate CO_2 molecule in a reactant state, respectively. Nafion has also been used to increase the proton conductivity to transport proton into the CO_2 reduction site of cathode for the one-pot reaction of the simultaneous electron/proton transfer. This system is expected to produce liquid solar fuel product with high solar to fuel efficiency ~0.2% in the PEC reaction.

Poster Presentation : **ENVR.P-574**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Ppy@rGO@CuFeO2-CuO@FTO multi-layer photocathode for photoelectrochemical(PEC) CO2 reduction.

Sangmun Han, Young soo Kang[1,*]

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

Global warming is one of the serious environmental issues that creates many disasters, including heat waves, floods, storms, and droughts. Among some greenhouse gases in the atmosphere, CO2 is considered as one of the most critical climate change gas. Photoelectrochemical (PEC) is a simple and effective method to reduce and convert CO2 gas into useful fuel, which will help to overcome global warming issues marginally. In this work, a multi-layered hybrid composite electrode of FTO/CuFeO2/CuO/rGO/PPy (polypyrrole) has been prepared as a photocathode for a smooth and effective CO2 reduction with FTO@BiVO4 as a photoanode. A hybrid composite of p-type semiconductors, CuFeO2@CuO has been chosen as cathode for CO2 reduction because of its narrow bandgap for visible light absorption and conduction band position which is suitable for CO2 reduction energy level. PPy has been selected to adsorb and activate a highly stable CO2 molecule. By considering the multi electron shuttling function to produce liquid solar fuels, rGO layers have been introduced as a functional layer of hybrid composite cathode. A structure of CuFeO2@CuO layer was confirmed by XRD and XPS, thickness of each layer was observed by SEM cross-section image. Electrochemical properties of each layer were studied and investigated by LSV, CV and EIS.

Poster Presentation : **ENVR.P-575**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Mixing behaviors and seasonal dynamics of total and methylated mercury in a shallow microtidal estuary: Hyeongsan River Estuary

Sangwoo Eom, Seunghee Han[1,*]

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

The biogeochemistry of total mercury (THg) and methylmercury (MeHg) was elucidated in Hyeongsan (HS) River estuary in Pohang City, South Korea. We focused on the estuarine mixing behaviors and seasonal dynamics of THg and MeHg in water and sediment. THg and MeHg were measured in HS River, Gumu Creek, and Chilsung Creek using cold vapor atomic fluorescence spectroscopy. The methylation rate constant (k_m) and acid volatile sulfide (AVS) analyses were proceeded to understand MeHg production rates and its controlling factors in sediment. The particulate Hg accounts for 81.4% of overall THg, which is higher than the particulate MeHg fraction (52.3%) in estuarine water. The distribution of particle-water partition coefficient (K_d) showed a large increase at the high salinity sites (> 20 psu), due to the salting out of dissolved Hg. The k_m in sediment was higher in the downstream than the upstream and Gumu Creek, and it was partially consistent with the distribution of AVS, implying that enhanced microbial activities and availability of mercury sulfide (HgS) are responsible for increased k_m in sediment. It was noted that typhoons considerably control sediment THg and MeHg dynamics, as was shown by the large loss of sediment and the consequent recovery of the concentrations during the following months. Moreover, MeHg input following the sediment disturbance by the typhoon was governed by the particle settling. We suggest that the spatiotemporal Hg dynamics are mostly affected by the transport of suspended particles associated with meteorological and hydrological conditions (e.g., rain depth, typhoon, and tidal current), and that qualifying transport of the particulate matter is critical to understand the fate of Hg in this estuary.

Poster Presentation : **ENVR.P-576**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

A strategy for improving the adsorption capacity of odor gaseous using thermal dried activated carbons

Sooyeol Phyo, Jiwon Lee[*]

Health and Welfare Research, Korea Institute of Science and Technology (KIST) / Division of Energy & Environment Technology, Korea University of Science and Technology (UST), Korea

Odor gaseous commonly generated in industrial field and living environment include a variety of of nitrogen containing odorous compounds (NOCs) such as ammonia, dimethylamine and trimethylamine. The thermal dried activated carbons (TDAC) were characterized and optimized for adsorption of various NOCs by precise control of the oxidation step. The granular activated carbons were used as the base carbon materials for the oxidation. The oxidation process in liquid phase were performed with nitric acid at 323K for 24 hr. Subsequently, the further oxidation conditions were precisely controlled by three different vacuum-drying temperature, resulting in different functional groups on the surface. The properties of the TDAC characterized by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS). The specific surface area were calculated by N_2/77K adesorption isotherms using the Brunauer-Emmett-Teller (BET) equation. To evaluate the NOCs adsorption capacity of TDAC, the breakthrough characteristics of the adsorbents were investigated using dynamic adsorption kinetic model. As a result, TDAC shows the higher adsorption capacity of ammonia, dimethylamine and trimethylamine adsorption capacities over the pristine activated carbon because of the hydrophilic groups on the surface. Furthermore, the competitive adsorption capacity and regeneration of NOCs adsorbed TDAC were demonstrated in this study.

Poster Presentation : **ENVR.P-577**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Highly sensitive gas sensor using graphene doped with ZnO nanosheets and SnO2 nano particles Centrifugated with CTAB for detection of NO2 gas

Lee Soyoung, Kang-Bong Lee[1,*], Yun Sik Nam[2]

Health and Welfare Research, Korea Institute of Science and Technology, Korea
[1]*Green City Technology Institute, Korea Institute of Science and Technology, Korea*
[2]*Advanced Analysis Center, Korea Institute of Science and Technology, Korea*

Highly sensitive gas sensor using graphene doped with ZnO nanosheets and SnO2 nano particles Centrifugated with CTAB for detection of NO2 gas So-young Lee1, 3, Yun-Sik Nam2, and Kang-Bong Lee1, 3*1 Center for Environment, Health and Welfare Research, Korea Institute of Science & Technology,Seoul, SeongBuk-gu, 136-791, South Korea2 Advanced Analysis Center and Green City Technonogy Institute, Korea Institute of Science & Technology,Seoul, SeongBuk-gu, 136-791, South KoreaFax: +82-(2)-958-5581 E-mail address: leekb@kist.re.krIn this work, single-layer graphene decorated with ZnO nanosheets and SnO2 nano particles for sensing NO2 gas has been demonstrated. The current research is focusing on the charateristic of ZnO nanosheets and SnO2 nano particles on graphene using spin coating technique for the fabrication of NO2 gas sensors. Physical properties for graphene composite doped with ZnO nanosheets and SnO2 nano particles have been intensively investigated using electron microscopy and various spectroscopies. Doping with ZnO nano sheets and SnO2 nano particles induced to change electronic properties of graphene, and it led to alter drastically resistivity of graphene in the presence of NO2 gas. ZnO nano sheets and SnO2 nano particles were centrifuged using CTAB as surfactants, which showed much faster recovery times compared to other surfactants (CTAC,PVP,Brij). Graphene doped with ZnO nano sheets and SnO2 nano particles demonstrated the ability to sense NO2 gas sensitively with the saturation time is around 200s, and with the limit of detection being below 0.15ppm. In comparison with other gases, to which the highest response was 40%, this sensor has very good selectivity and repeatedly.

Poster Presentation : **ENVR.P-578**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Development of an ultrasensitive colorimetric detection method of dichromate ions with a colorimetric sensor based on gold nano flower particles

Sujin Yoon, Yun Sik Nam[1], Kang-Bong Lee[*]

Center for Environment, Health and Welfare Research, Korea Institute of Science and Technology, Korea
[1]*Advanced Analysis Center, Korea Institute of Science and Technology, Korea*

A simple and facile colorimetric method for the detection of dichromate ions using flower-shape gold nanoparticles (AuNFs) has been developed. Herein, a novel approach method was developed, based on the measurement of localized surface plasmon resonance absorption. Addition of dichromate ions selectively induced the aggregation of flower-shape gold nanoparticles, which resulted in red-shifted absorption accompanied by a color change from magenta purple to pale blue. The binding site and sensing mechanism for dichromate ions flower-shape gold nanoparticles were characterized by Fourier Transform infrared spectroscopy, ultraviolet-visible spectroscopy, and transmission electron microscopy. The optimized detection of dichromate ions via the flower-shape gold nanoparticle-based probe occurred at pH 4.0 and 30 □C. The absorption ratios (A800 nm/A575 nm) were proportional to the dichromate ions concentrations within the range 0.0 μM–1.1 μM, with a detection limit of 3.03 nM in tap and pond water, respectively. The highly selective and sensitive colorimetric assay reported herein has been successfully applied to monitor the dichromate ionsconcentrations in spiked tap water, pond water samples. This sensing system allows rapid and facile determination of dichromate ions in various types of mineral supplement, and environmental samples.

Poster Presentation : **ENVR.P-579**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Highly selective detection of Iodine based on gold nano-dahlia

Hana Park, Yun Sik Nam[1], Kang-Bong Lee*

Health and Welfare Research, Korea Institute of Science and Technology, Korea
[1]*Advanced Analysis Center, Korea Institute of Science and Technology, Korea*

Iodine is not only an essential mineral of human body but also used to various field such as food, medical, and industry. However, high iodine intakes can also cause thyroid disease and burning of the mouth, throat, and stomach. In this study, we investigated on an Iodine colorimetric sensor based on Dahlia shaped gold nanoparticles(GND). Gold nanoparticles are studied for variety of applications including sensor by their unique optical properties. However, pristine gold nanoparticles should have functionalization due to their low sensitivity and poor dynamic range. This issue is overcome by simple method as a change their shape. The etching of GND occurred by Iodide ion selectively. Due to the bump became invisible, the color changes from blue to pink. The optimized condition of GND is performed at pH 5.0 and 60 ℃. Here, we demonstrate that gold nano-dahlia(GND) can be used to detecting Iodine in different water samples by colorimetric sensor. Thereby we suggest the way to highly selective detecting Iodine more easily and portable.

Poster Presentation : **ENVR.P-580**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Photocatalytic and electrocatalytic properties of Eu(III)-doped perovskite $ZnGa_2O_4$ nanoparticles with dopant level approaches

Hye Ji Jang, Youngku Sohn[*]

Department of Chemistry, Chungnam National University, Korea

Spinel $ZnGa_2O_4$ has shown high activities in many photocatalytic application areas. Herein, Eu(III)-doped $ZnGa_2O_4$ nanoparticles were synthesized by the hydrothermal method. The morphologies, microstructures and photoluminescent properties were analyzed by scanning electron microscopy, high resolution transmission electron microscopy, X-ray photoelectron spectroscopy (XPS), and photoluminescence spectroscopy. Photocatalytic CO_2 reduction tests were performed under UVC and UVB light. To evaluate the photo-electrochemical oxygen evolution performances, the linear sweep voltammograms were acquired under 395nm light irradiation. The demonstration results have shown that Eu(III) dopant plays a significant role in the photocatalytic CO2 reduction and (photo)electrochemical oxygen evolution reaction performances.

Poster Presentation : **ENVR.P-581**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Electrochemical CO_2 conversion over brass substrates

Hong Sung-min, Youngku Sohn[1,*]

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

The electrochemical conversion of carbon dioxide into chemical fuels has been considered as a potential strategy to reduce excess CO_2 levels in the atmosphere. Herein, brass (Cu-Zn) has been demonstrated as a potential electrocatalyst for electrochemical CO_2 reduction. Amperometry has been conducted in an 0.1 M $NaHCO_3$ electrolyte at different applied potentials. Gaseous and liquid CO_2 reduction products have been examined by gas chromatography and nuclear magnetic resonance spectroscopy, respectively. The catalytic performances were discussed with the physiochemical properties by scanning electron microscopy, X-ray photoelectron spectroscopy, Raman, and X-ray diffraction crystallography before and after the CO_2 reduction tests.

Poster Presentation : **ENVR.P-582**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Synergistic effects of nanoclay and hydrolysis on performance of polyacrylonitrile membrane for pervaporative desalination of brine

Hasan Fareed, Ghulam Hussain Qasim[1], Seunghee Han[2,*]

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

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

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

Pervaporation (PV) is a well-developed technique for efficient separation of azeotropic mixtures, and it is now slowly but steadily proving its potential in the domain of desalination owing to its unimpaired rejection of monovalent ions. However, the exceptional salt rejection of PV comes at the cost of reduced flux because of the use of dense selective layer. In this study, the kaolin was blended in polyacrylonitrile (PAN) matrix followed by a controlled alkaline hydrolysis reaction to enhance the membrane flux and durability without compromising on salt rejection. The hydrolyzed mixed matrix membranes were prepared by mixing varying amount (2-10%) of kaolin with PAN and casting them using non-solvent induced phase separation technique. All the membranes were hydrolyzed in alkaline solution to further improve the physiochemical properties. A 2% kaolin loading resulted in well-developed profile of membrane resulting in superior hydrophilicity, increased flux and improved mechanical strength. Hydrolysis reaction caused dramatic increment of hydrophilic carboxylic functional groups while the mechanical strength was compromised slightly. Hydrolyzed membrane with 2% kaolin dosing exhibited superlative flux of 82 and 59 kg m^2 h^{-1} for 3.5 and 10% NaCl feed solution, respectively, at 65°C feed temperature while maintaining salt rejection above 99.9%. The developed membrane also proved its reliability when it was endured through continuous filtration mode (72h) for brine desalination by sustaining a stable flux and salt rejection.

Poster Presentation : **ENVR.P-583**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Improvement of the Mechanical Properties of Recast Perfluorinated Polymer Electrolyte Membranes by Annealing

Mahamuda Akter , Beom-Seok Kim[1], Jong-Hyeok Park[2], Jin-Soo Park[1,*]

Department of Civil, Environmental, and Biomedical Engineering, Sangmyung University, Korea
[1]*Department of Green Chemical Engineering, Sangmyung University, Korea*
[2]*Department of Civil, Environmental, Korea*

Fuel cells are electrochemical devices that convert chemical energy into electrical energy via anodic and cathodic reactions. A unit cell of proton exchange membrane fuel cells contains two electrodes, e.g., an anode and a cathode, and a proton exchangeable electrolyte which is partitioned the anode from the cathode. Perfluorosulfonic acid (PFSA) membranes are commonly used in proton exchange membrane fuel cells, which are classified with a long side chain and a short side chain. Presently, two types of solution-cast membranes were produced from commercially available PFSA ionomers and lab-made PFSA ionomers developed by the Korea Research Institute of Chemical Technology. The ionomer dispersion has been molded on the glass plate and dried overnight at 60 oC into the convective oven for removing solvents under the vacuum condition. The effect of annealing of recast membranes on their properties were investigated with the respect of annealing temperature and annealing number. All the recast membranes have been characterized in terms of high proton conductivity, water uptake (WU), and ion exchange capacity (IEC). In addition, we have discussed the effect of annealing temperatures on the crystalline size, crystallinity, mechanical strength, crossover current, and proton conductivity.AcknowledgmentThis work was supported in part by the New and Renewable Energy of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) granted financial resource from the Ministry of Trade, Industry & Energy, Republic of Korea (No. 20193010032480) and by 2021 Green Convergence Professional Manpower Training Program of the Korea Environmental Industry and Technology Institute funded by the Ministry of Environment.

Poster Presentation : **ENVR.P-584**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Correlation of Thickness of Ionomer Film with the Performance of PEMFCs

Jong-Hyeok Park, Beom-Seok Kim[1], Jin-Soo Park[1,*]

Department of Civil, Environmental, and Biomedical Engineering, Sangmyung University, Korea
[1]*Department of Green Chemical Engineering, Sangmyung University, Korea*

Proton exchange membrane fuel cells (PEMFCs) require the movement of protons generated and consumed at anode and cathode (so called, catalyst layers) respectively. Protons should be transported at catalyst layers to participate in anodic and cathodic reactions. Among various proton conductors, proton exchange ionomers are quite often chosen, mostly perfluorosulfonic acid ionomers. The technique to introduce ionomers in catalyst layers for oxidation and reduction reactions in PEMFCs is the preparation of catalyst inks consisting of solid electrocatalyst, liquid ion exchangeable ionomer dispersion, additional solvents and additives along with the evaporation of all solvents in catalyst inks. Various solvents in dispersions cause different shapes of ionomers such as cylindrical rods, a less-defined large particles, coils, and so on. Such different types of ionomers are subject to form distinguished thickness of ionomer and structure catalyst layers, which causes the different performance of PEMFCs. In this study, we investigate the correlation of ionomer properties film with the performance of PEMFC. Electrochemical characterization, x-ray photoelectron spectroscopy, ellipsometry, and contact angle were carried out to figure out the correlation.AcknowledgmentThis work was financially supported in part by the New and Renewable Energy of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) granted financial resource from the Ministry of Trade, Industry & Energy, Republic of Korea (No. 20193010032480) and by 2021 Green Convergence Professional Manpower Training Program of the Korea Environmental Industry and Technology Institute funded by the Ministry of Environment.

Poster Presentation : **ENVR.P-585**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Effect of Property of Ionomer Dispersion on Catalyst Layers for Hydrogen Evolution Reaction in PEMWE

Jong-Hyeok Park, Beom-Seok Kim[1], Jin-Soo Park[1,*]

Department of Civil, Environmental, and Biomedical Engineering, Sangmyung University, Korea
[1]*Department of Green Chemical Engineering, Sangmyung University, Korea*

Proton exchange membrane water electrolysis (PEMWE) consists of two different catalyst layers to complete the full electrochemical reactions. The movement of protons generated and consumed at anode and cathode, respectively, is one of the important mass transport phenomena in catalyst layers. Among proton conductors for hydrogen evolution reaction electrode, proton exchange ionomers are quite often chosen, mostly perfluorosulfonic acid ionomers. The technique to introduce ionomers in catalyst layers for oxidation and reduction reactions in PEMWE is the preparation of catalyst inks consisting of solid electrocatalyst, liquid ion exchangeable ionomer dispersion, additional solvents and additives. Various solvents in dispersions cause different shapes of ionomers. Such different types of ionomers are subject to form distinguished thickness of ionomer and structure catalyst layers, which causes the different performance and durability of PEMWE. In this study, the effect of solvents dispersing ionomers on the performance and durability of catalyst layers was investigated. Electrochemical characterization such as I-V polarization, cyclic voltammetry, impedance, and so on and microscopic characterization such as SEM and TEM were carried out to evaluate the performance and durability of catalyst layers in PEMWE.AcknowledgmentThis research was financially supported in part by the Hydrogen Energy Innovation Technology Development Program of the National Research Foundation (NRF) funded by the Ministry of Science, ICT & Future Planning(NRF-2019M3E6A1063677) and by 2021 Green Convergence Professional Manpower Training Program of the Korea Environmental Industry and Technology Institute funded by the Ministry of Environment.

Poster Presentation : **ENVR.P-586**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Visible activation of humic acid–TiO_2 complex mediated via ligand-to-metal charge transfer

Hoang Tran Bui, EunJu Kim[1,*], Wooyul Kim[2,*]

Department of Chemical and Biological Engineering, 숙명여자대학교, Korea
[1]*Korea Institute of Science and Technology, Korea*
[2]*Department of Chemical and Biological Engineering, Sookmyung Women's University, Korea*

TiO_2 is a popular material that is widely utilized in various application fields such as cosmetics, pigments, catalysts, solar cells, etc., therefore, its release to the natural environment, especially the aquatic ecosystem increases progressively with time. The complexation of dissolved organic matter (DOM) with TiO_2 conceivably occurs when the TiO_2 consistency reaches the appropriate proportion. Herein, we exhibit that humic acid-adsorbed TiO2 (HA/TiO_2) performs photoactivity under visible light through ligand-to-metal charge transfer (LMCT). The generation of H_2O_2 via the conduction band is proved to contribute to pollutant removal and bacterial inactivation under visible light irradiation. Simultaneously, we find the key role of the phenolic group in visible light absorption and H_2O_2 photogeneration between TiO_2 NPs and HA among the organic functional groups in HA. TiO_2 at environmentally relevant and supra-environmental concentrations is spiked in the realistic river water to evaluate the additional contribution of LMCT-mediated yield to naturally occurring H_2O_2 generated from background organic constituents. Our findings suggest that H_2O_2 generation by HA/TiO_2 is related to the quantity and functional group chemistry of DOM, which informs the H_2O_2-induced toxic effects on aquatic species in surface waters.

Poster Presentation : **ENVR.P-587**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Electrocatalytic CO_2 reduction over perovskite oxide catalysts

Ju Hyun Yang, Youngku Sohn[1,*]

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

Perovskite oxide has shown potential application in electrocatalytic CO_2 reduction. Herein, perovskite oxides were synthesized by the hydrothermal method and evaluated their electrocatalytic activities. Their physicochemical properties were characterized by scanning electron microscopy, X-ray diffraction crystallography, high resolution transmission electron microscopy, and X-ray photoelectron spectroscopy. For the evaluation of the catalytic activity, amperometry and gas chromatography tests were conducted to confirm CO_2 reduction products of CO, CH_4 and some C_n compounds. The present results provide useful information on the application of perovskite oxides to electrocatalytic CO_2 reduction for energy recycling.

Poster Presentation : **ENVR.P-588**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Removal of aqueous cesium by prussian blue embedded pectin beads synthesized from steel slag

Sunho Yoon, Sungjun Bae[1,*]

Environmental engineering, Konkuk University, Korea
[1]*Department of Environmental Engineering, Konkuk University, Korea*

Prussian blue (PB) is one of the potential materials, which could be applied as selective cesium (Cs^+) adsorbent because its crystal lattice has a cage size similar to the radius Cs^+. However, the small particle size of PB limits its direct application because the particles rapidly disperse in aqueous system, which make difficult to separate or recover them from the water after use as an adsorbent. Therefore, the immobilization of PB on supporting materials has steadily progressed toward application as a practical water treatment process. In this study, we developed PB embedded pectin bead (PB@PD) synthesized from Fe and Ca sources in steel slag (SS). A variety of surface analysis such as X-ray diffraction, x-ray photoelectron spectroscopy, scanning electron microscope, and Fourier transform infrared were carried out to characterize the PB@PD. Batch adsorption test conducted using PB@PD revealed that the maximum adsorption capacity of Cs^+ was 54 mg/g. In addition, PB@PD could be recycled up to 4 times and was very effective for Cs^+ adsorption in artificial seawater. Finally, we applied the PB@PD as filling material in a fixed-bed column reactor for continuous Cs^+ removal, showing the remarkable adsorption capacity without any clogging problem during the Cs^+ treatment. **Acknowledgments**: This research was supported by the National Research Foundation of Korea (2019R1C1C1003316) and the Korea Environment Industry & Technology Institute (KEITI) through “Subsurface Environmental Management (SEM) Project”, funded by Korea Ministry of Environment (MOE) (2020002480006), and the Konkuk University Researcher Fund in 2020.

Poster Presentation : **ENVR.P-589**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Various synthesis method and comparison of photoelectrochemical efficiency for $BiVO_4$ / Spaced TiO_2 nanotubes heterojunction

Taewan Kim, Kiyoung Lee*

Department of Chemistry and Chemical Engineering, Inha University, Korea

After the discovery of TiO_2 photoelectrochemical water electrolysis reported by Fujishima and Honda in 1972, research on water electrolysis using TiO_2 has been actively conducted. TiO_2 has a bandgap energy of 3.0-3.2 eV and is a semiconducting material that responds to light in the ultraviolet region below 400 nm. However, since ultraviolet light is only about 4 % of the total light, there is a limit to practical application of TiO_2 as a single material. $BiVO_4$ has the advantage of being able to absorb light in the visible region below 563 nm with a low band gap of 2.2 to 2.4 eV, non-toxicity and excellent stability. However, $BiVO_4$ has the main disadvantage of a high electron-hole pair recombination rate of 60–80% due to low electron transfer. These disadvantages can be offset by contact with the excellent electronic properties of TiO_2 nanotubes, and light in the ultraviolet and visible regions can be used for heterojunctions. For this reason, an increase in photoelectrochemical efficiency can be expected when a heterojunction between TiO_2 nanotubes and $BiVO_4$. In the case of a typical TiO_2 nanotube structure, as the thickness of the coating was increases, it will be blocking the hole of tubes. This phenomenon is a factor that lowers the photoelectrochemical efficiency. In this study, we use spaced TiO_2 nanotubes which has hollow spaced between tube and tubes by controlling the anodization conditions to facilitate $BiVO_4$ heterojunctions and we presented various synthetic methods for fabricated $BiVO_4$/TiO_2heterojunction. It was confirmed that the photoelectrochemical efficiency of the $BiVO_4$ heterojunction structure coated in the sufficient space between the TiO_2 nanotubes was improved due to the larger surface area and the optimized $BiVO_4$ thickness compared to the general nanotube structure.

Poster Presentation : **ENVR.P-590**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

High-Performance Small-Molecule Based Organic Photovoltaics through Strategic Halogenation

Seung Un Ryu, Hyuntae Choi, Taiho Park*

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

In this study, a series of benzodithiophene (BDT)-based active materials substituted with specific halogen atoms were designed and synthesized to control the morphology of photoactive layer. The effect of these strategies on the bulk-heterojunction (BHJ) morphology is systematically investigated through microstructure analyses (GIWAXS). In particular, the small-molecule substituted with chlorine atoms (BDTID-Cl) exhibits well-mixed morphology and interpenetrating networks when blended with $PC_{71}BM$. These morphological features allow efficient charge transport, resulting in the outstanding performance with a power conversion efficiency (PCE) of 10.5% and the highest fill factor (FF) of 78.0% in the single-junction small-molecule based organic photovoltaics. Moreover, the two-terminal (2T)-tandem organic photovoltaics achieve an excellent PCE of 15.1% through complementary absorption and favorable morphology in the photoactive layer. These results provide the valuable insight that tailoring molecular interactions via halogenation is an effective approach to control BHJ morphology and achieve remarkable performance in small-molecule based organic photovoltaics.

Poster Presentation : **ENVR.P-591**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Formation of Ni-Fe Heterostructures through the one-step electro deposition method to improve water electrolysis performance

Jaewon Lee, Kiyoung Lee*

Department of Chemistry and Chemical Engineering, Inha University, Korea

In the past decades, research on renewable energy has been intensively studied. Among several renewable energies, hydrogen energy has been considered the most promising energy resources due to its high energy density, clean energy source. Electrolysis has been considered the cleanest and most industrially applicable approach. In general, noble metal such as Pt, Ir, and Ru are currently used for catalysts in efficient water electrolysis. However, these materials are expensive. Therefore, many studies have been focused on replacing to inexpensive materials like transition metal or metal oxide. In particular, nickel compounds such as nickel oxide, nickel sulfide have the excellent water electrolysis efficiency except for precious metal. In our research group, Ni-Fe heterostructures were fabricated by simple one-step electrodeposition method. The surface structure was adjusted by controlling the concentration of coagulant such as NH_4F, thiourea during electrodeposition process. Morphological characterization was analyzed using SEM, EDX, XRD and electrochemical analysis such as OER, EIS were performed using potentiostat. The microshape structure resulted from electrodeposition provide a large surface area and shows overpotential of 238 mV at 10 mA/cm^2 and chare transfer resistance of about 0.5 Ω.

Poster Presentation : **ENVR.P-592**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Removal behavior of microplastics in drinking water treatment processes

Sang-Heon Na, EunJu Kim*

Water Cycle Research Center, Korea Institute of Science and Technology, Korea

The massive use of plastic products and inadequate management of plastic wastes lead to microplastics being ubiquitously found in rivers and lakes that are the main sources for drinking water in Korea. The effectiveness of traditional drinking water treatment plants for the removal of microplastics in the size range of tens of micrometers is currently uncertain. Herein this study investigated the behavior and removal efficiency of four different sized polystyrene microplastics (10−90 μm in diameter) in a simulated cascade of coagulation/sedimentation, sand filtration, and UV-based oxidation. The results showed that the larger the particle size of microplastics, the higher the removal efficiency was during coagulation and sand filtration. Approximately 16% of 10 μm microplastics injected passed through the sand, which were further fragmented by UV oxidation. UV/H2O2 treatment promoted the MP fragmentation and chemical leaching more significantly than UV treatment, resulting in a higher toxicity for UV/H2O2-treated water. Our findings pave the way for deeper understanding of how microplastics behave and transform in a sequential drinking water treatment process.

Poster Presentation : **ENVR.P-593**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Study on Photoelectrochemical Hydrogen Evolution of (1 0 1) Facet Single Crystalline TiO_2 onto $WO_3/BiVO_4$ Heterojunction

Sanghyeon Moon, Kiyoung Lee*

Department of Chemistry and Chemical Engineering, Inha University, Korea

Producing hydrogen (H_2) via photoelectrochemical (PEC) water splitting is a way of converting solar energy to H_2, one of the greatest approaches to overcome energy problems. $WO_3/BiVO_4$ heterojunction has been studied widely in PEC water splitting branch due to type II band alignment. In type II band alignment of $WO_3/BiVO_4$ heterojunction, valance band and conduction band edge positions of $BiVO_4$ possesses more negative than WO_3, photogenerated electrons are inject into conduction band of WO_3. Moreover, photogenerated electrons can easily transfer through the conduction band of WO_3 to current collector. However, $WO_3/BiVO_4$ heterojunction shows poor stability because of V^{5+} leaching from $BiVO_4$ during PEC operations. Herein, we have demonstrated facile synthesis of coating (1 0 1) facet single crystalline TiO_2 onto $WO_3/BiVO_4$ heterojunction by hydrothermal and spin-coating method, which leads to improve the photocatalytic performance. The coated (1 0 1) facet single crystalline TiO_2 layer acts as blocking surface defects within enhancing electron-hole separation, corrosion resistance and photostability. Fabricated $WO_3/BiVO_4/TiO_2$ heterojunction allows 4.5 times higher PEC performance and 2.1 times higher H_2 production rate than pristine WO_3 nanoplates under simulated solar light irradiation. Further, it showed excellent quantum efficiency (45% at 460 nm) and long-term photostability (24 h).

Poster Presentation : **ENVR.P-594**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Electrochemical CO_2 reduction over modified CuS electrodes

Minhee Joo, Youngku Sohn[1,*]

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

The daily CO_2 level increase by consumption of hydrocarbon fuels is becoming more serious. To minimize the impact from CO_2, capture and CO_2 energy conversion have extensively been researched and applied. Herein, we have demonstrated electrochemical CO_2 energy conversion over developed modified CuS electrodes. The conversion products are gases and liquids that are analyzed by gas chromatography and nuclear magnetic resonance spectroscopy, respectively. Faradaic efficiency and selectivity are evaluated at different applied potentials. The catalytic conversion activities are discussed with the physicochemical properties by X-ray photoelectron spectroscopy, X-ray diffraction crystallography (XRD), scanning electron microscopy, transmission electron microscopy, and Raman spectroscopy.

Poster Presentation : **ENVR.P-595**

Environmental Energy

Exhibition Hall 1 THU 11:00~12:30

Noble Metal Sensitized Invasive Porous Bioelectrodes: Advanced Medical Device for Enhanced Neuronal Activity and Chronic Alcohol therapy

Hong Soo Kim, **Su Il In**[1,*]

Department of Energy Science and Engineer, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Energy Systems Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

The use of invasive bioelectrodes has long been accepted as an effective treatment modality for a variety of conditions. Modern invasive bioelectrodes are generally fabricated from stainless steel because of their relatively low cost, ease of fabrication, and high biocompatibility, thus are inserted at specific points in the body for treatment. While the underlying biological mechanism of invasive bioelectrode treatment remains as yet undetermined, it has been largely accepted that the inserted bioelectrode interacts mechanically and electrochemically with the surrounding tissue, thus altering the neurochemical balance of the peripheral and central nervous systems. In this study, we first report, to the best of our knowledge, the novel development of invasive porous bioelectrodes sensitized with noble metal nanoparticles, as well as the detailed characterization of their electrophysiological effects on neuronal activity and their use in treating chronic alcoholism. Using an in vivo Sprague-Dawley rat model, we find the noble metal sensitized porous bioelectrodes, compared to conventional bioelectrodes as well as unsensitized invasive porous bioelectrodes, exhibit significantly improved electrophysiological neuronal activity. In particular, silver nanoparticle sensitized invasive porous bioelectrodes (Ag-IPB) show high alcohol detoxification with bioelectrode stimulation. We believe this to be the first report of noble metal sensitized invasive porous bioelectrodes showing enhanced neuronal activity and a substantial alcohol detoxification effect.

Poster Presentation : **ENVR.P-596**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Noble metal free photocatalyst: TiO_2 NTs covered with rGO

Dongyun Kim, **Su Il In**[*]

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

TiO_2 nanotube arrays (TNT) are the subject of great current interest among the photocatalysis research, however the relatively large band gap that provides TiO_2 with its excellent corrosion stability severely limits its absorption of solar spectrum energy To increase the optical absorption of TiO_2 while maintaining its otherwise commendable properties several approaches have been investigated including doping with non-metal or noble metal co-catalysts such as Pt and coupling with low band gap semiconductors With the aim of replacing expensive noble metal co-catalysts, we report a noble metal-free novel nanostructured photocatalytic material fabricated using a facile synthesis approach, comprising a one dimensional array of TNT covered with a reduced graphene oxide-TiO_2 nanoparticles (rGO-TiO_2 NP) composite The novel nanostructure exhibits significantly improved photocurrent density and photochemical activity via conversion of CO_2 into methane under simulated solar light irradiation The improved performance appears because of the combined effect of enhanced light absorption and effective charge separation promoted by the rGO.

Poster Presentation : **ENVR.P-597**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Design and Fabrication of the Dye-sensitized Betavoltaic Cell using Isotope Carbon Nanoparticle

Hong Soo Kim, Su Il In[1,*]

Department of Energy Science and Engineer, Daegu Gyeongbuk Institute of Science & Technology, Korea
[1]*Department of Energy Systems Engineering, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Betavoltaic cells, similar in concept to a photovoltaic cell, combine a beta radiation source with a p–n junction semiconductor couple. The beta radiation impinges on the semiconductor p–n junction, thereby exciting the valence band electrons into the conduction band. The useful life time of a betavoltaic device depends upon the half-life of the isotope; with tritium, for example, it can be used for at least 10 years. A critical factor influencing betavoltaic performance is the radioisotope, like H-3, Ni-63, S-35, and Pm-147, each of which have their own energy density and half-life, which are inversely related. The first betavoltaic cell was reported by Paul Rapport in 1953; the cell, fabricated utilizing Sr90–Y90 as a radioactive source, exhibited an efficiency of 0.2%. Several researchers have explored semiconductor materials such as SiC, GaN, and GaAs to improve conversion efficiencies. Cheng and co-workers fabricated betavoltaic cells using nanotubes of graphene-TiO2, and black titania. Herein, we report on a dye-sensitized betavoltaic cell (DSBC), a new addition to aforementioned technologies, which successfully integrates two different technologies: dye-sensitized photovoltaics and beta particle excitation. In this device, carbon-14 (C-14) is concurrently used as the beta particle source and the counter electrode. In contrast with semiconductor-based betavoltaic cells, the operation of a DSBC depends on beta radiation exciting surface-bound dye molecules.

Poster Presentation : **ENVR.P-598**
Environmental Energy
Exhibition Hall 1 THU 11:00~12:30

Application of Re-use Graphite Recycled from the Spent Lithium-Ion Batteries for Highly Stable Lithium-Sulfur batteries

Sungyool Bong, Jaeyoung Lee[1,*]

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

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

Demand for electronic devices and electric cars has been significantly increasing of late. Consumption of portable electronics - laptops, mobile phones, tablets, digital cameras, camcorders, portable chargers, and wearable devices - has also been rising rapidly due to the improvement in the standard of living and growth in disposable income of consumers across the globe. Significantly, the automotive market is dramatically increasing the use of rechargeable batteries with a lifespan of around five to ten years, depending upon the size and type of batteries. Batteries are replaced with new ones at the end of their lifespan. Old batteries are sent for the recycling process. Several electric and car manufacturing/material production companies have started recycling batteries. Therefore, the rise in demand for portable electronic devices/electric automotive is anticipated to provide immense opportunities to the battery recycling market during the forecast period.In this trend, the battery recycling process is essential for the environmental and renewable energy fields. There are several recycling parts, such as plastic frames, metal electrodes, and carbons in the spent batteries. Several research papers have reported recycling materials in lithium-ion batteries; however, they have been seldom applied in lithium-sulfur batteries. In this presentation, we report applications for graphite materials for lithium-sulfur batteries from the spent lithium-ion batteries. The characterization and electrochemical results depend on the experimental factors - removal of metal impurities and high-temperature treated process.