

Plenary Lecture : **PLEN-1**

Plenary Lecture

Room 304 (Live Streaming) WED 11:00

Chair: Dongwhan Lee (Seoul National University)

Targeted Protein Degradation – Challenges and Opportunities

Gray Nathanael S.

Chemical and Systems Biology at Stanford, United States

Targeted protein degradation (TPD) refers to the use of small molecules to induce ubiquitin-dependent degradation of proteins. These degrader molecules are of great interest in drug development as they can address previously inaccessible targets. However, degrader discovery and optimization remains an inefficient and empirical process due to a lack of understanding of the key molecular events required to successfully induce target degradation. In this seminar I will discuss the use chemo-proteomics to annotate the ‘degradable kinome’. This work will not only fuel kinase degrader discovery, but also provides a blueprint for evaluating targeted degradation across entire gene families, to accelerate understanding of TPD beyond the kinome.

Award Lecture : **AWARD-1**

Award Lecture

Room 304 (Live Streaming) FRI 11:30

Nonadiabatic Reaction Dynamics in the Excited States of Polyatomic Molecules

Sang Kyu Kim

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

Nonadiabatic dynamics are ubiquitous in nature. We are going to introduce some unique examples where we could interrogate nonadiabatic transition processes at the molecular level in both spatial and temporal domains. Photo-induced processes such as predissociation, tunneling, nonradiative transitions and photo-detachment are driven by the nonadiabatic transitions especially in the vicinity of conical intersections. As the conical intersection is multi-dimensional in nature, it is not straightforward to define the strong coupling region by any means. We demonstrate that it is possible to prepare the reactive flux in the proximity of the conical intersection volume to unravel the detailed nonadiabatic bifurcation dynamics mechanism in molecular details. Various experimental tools such as resonant-enhanced ionization, Stark-deflection, hole-burning, IR+UV double resonances, (slow) velocity-map ion/electron imaging (VMI), or picosecond/femtosecond time-resolved pump-probe VMI have been employed to investigate the microscopic mechanism of the excited-state chemistry of neutrals and anionic species prepared at the low temperature of 1 - 35 K. Here, we are going to show how we could possibly characterize structures of the conical intersections or transition states where the molecule stays only briefly in the respective $(3N-8)$ or $(3N-7)$ normal mode space where N is the number of atoms in polyatomic systems.

References:

- [1] J. S. Lim, H. S. You, S. Y. Kim, S. K. Kim, Chem. Sci. 2019 10 2404.
- [2] K. C. Woo and S. K. Kim, J. Phys. Chem. A 2019 123 1529.
- [3] H. S. You et. al., J. Phys. Chem. A 2018 122 1197.
- [4] K.-C. Woo, D. H. Kang, and S. K. Kim, J. Am. Chem. Soc. 2017 139 17152.
- [5] H. S. You et. al. Int. Rev. Phys. Chem. 2015 34 429.
- [6] H. S. You et. al., J. Phys. Chem. Letters 2015 6 3202.
- [7] J. Lim and S. K. Kim, Nat. Chem. 2010 2 627.

[8]D. H. Kang, S. An and S. K. Kim, Phys. Rev. Lett. 2020 125 093001.

[9]K. C. Woo and S. K. Kim, J. Phys. Chem. Lett. 2020 11 6730.



Symposium : **KCS1-1**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 14:00

Chair: Cheol-Hong Cheon (Korea University)

Progress in Enantioselective Gold Catalysis

Seunghoon Shin

Department of Chemistry, Hanyang University, Korea

Over the past two decades, homogeneous gold catalysis has generated numerous useful synthetic tools, which can be traced to its unparalleled ability to activate pi-bonds toward nucleophilic additions. Enantioselective gold catalysis has also evolved along the way, but at a much slower pace. Linear dicoordination geometry of Au(I) complexes impose the approach of pronucleophiles from the opposite side of the chiral ligand, which presents especially severe challenge in the intermolecular reactions. Herein, we discuss two examples of asymmetric intermolecular reaction involving propiolates. One is the [4+2] annulation between propiolates and alkenes, leading to formation of optically enriched dihydropyranones.¹ Appropriate choice of solvents as well as the use of SDS (surfactant) was pivotal in obtaining high enantioselectivity. Second example is the reaction of propiolates with allyl (thio)ethers, involving enantioselective Claisen rearrangement.² Problems such as low stereoselectivity and the dissociation of allyl cation could be overcome by adopting thioethers. References 1. Kim, H.; Choi, S. Y.; Shin, S. *Angew. Chem. Int. Ed.* 2018, 57, 13130. 2. Kim, H.; Jang, J.; Shin, S. *Gold(I)-Catalyzed Asymmetric Thioallylation of Propiolates via Charge-Induced Thio-Claisen Rearrangement.* *J. Am. Chem. Soc.* 2020, 142, 20788.

Symposium : **KCS1-2**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 14:20

Chair: Cheol-Hong Cheon (Korea University)

Ni-Catalyzed Heterocycle Synthesis

Eun Jin Cho

Department of Chemistry, Chung-Ang University, Korea

We have developed synthetic methods for various heterocycles by exploiting the different reactivity pattern of Nickel depending on its oxidation state. Ni(II) has the potential to undergo transmetalation with boronic acid derivatives followed by arylation of alkynes to give alkenyl Ni-intermediate which can act as nucleophile reacting with carbonyls. In the presence of Ni(II) salts, multi-functionalized benzofurans and indoles have been synthesized from alkyne-tethered phenolic esters and acetamide derivatives, respectively. Furthermore, this methodology could be extended to the synthesis of tetracyclic 6H-isoindolo[2,1-a]indol-6-ones from phenyl acetylenes containing 2-phenyl phthalimide. Notably, the presence of extended conjugation at 11-position of 6H-isoindolo[2,1-a]indol-6-ones imparted it fluorescence phenomena to be used as new organophotocatalysts. On the other hand, Ni(0) has ability to undergo oxidative insertion to form Ni(II), forming a five membered nickelacycle. A synthetic route for accessing multifunctionalized indoles was developed through Ni(0)-catalyzed transcarboamination using 2-alkynylanilinoacrylate. C–N bond cleavage of a nickelacycle intermediate and syn/anti-rotation of the alkenyl-Ni intermediate are the key steps of this transcarboamination. In addition, this Ni(0) chemistry could be utilized for an exogenous base-free procedure of a stereoselective arylvinylation of alkynes. It was revealed that Ni(0) species generated in situ from air-stable Ni(II) precursor by a P[^]N ligand undergoes oxidative cyclization with an unactivated enyne to afford a nickelacycle intermediate, where a B-assisted C–O bond cleavage results in the formation of TM-active boronate complex affording tetrasubstituted 1,3-diene products stereoselectively.

Symposium : **KCS1-3**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 14:40

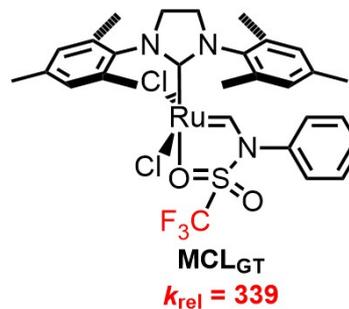
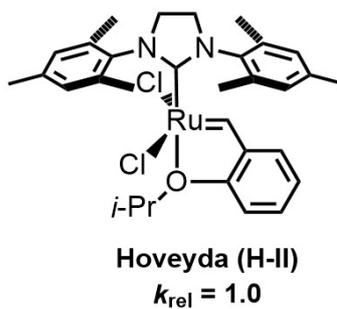
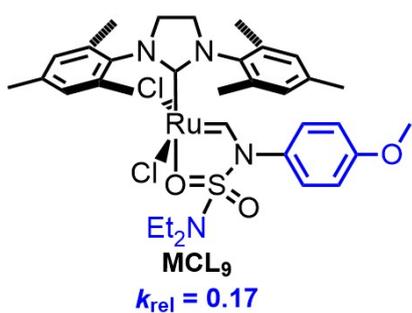
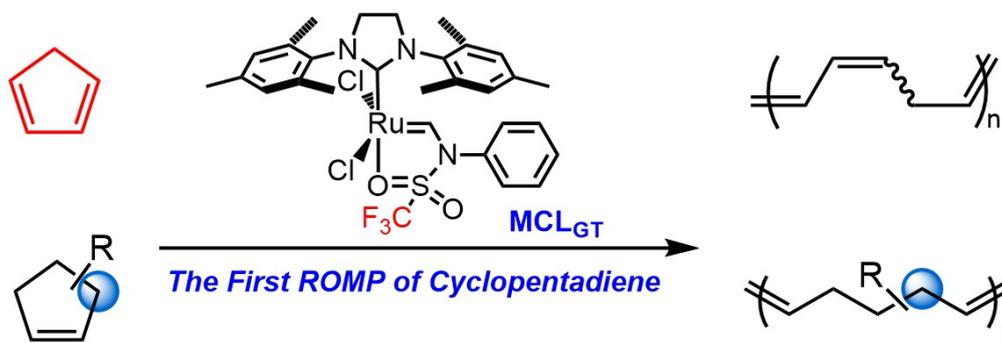
Chair: Cheol-Hong Cheon (Korea University)

Highly Active Ruthenium Olefin Metathesis Catalysts Enabling Ring-Opening Metathesis Polymerization of Low-Strained Cyclic Olefins

Soon Hyeok Hong

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

Highly controllable ruthenium catalysts were developed using readily available and versatile N-vinylsulfonamides as carbene precursors. Catalyst initiation rates were controlled in a straightforward manner, from latent to fast initiating, through the facile modulation of the N-vinylsulfonamide ligands. Trifluoromethanesulfonamide-based catalysts initiated ultrarapidly even at temperatures as low as $-60\text{ }^{\circ}\text{C}$ and continuously propagated rapidly, enabling the enthalpically and entropically less-favored ring-opening metathesis polymerizations of low-strained functionalized cyclopentene derivatives, some of which are not accessible with previous olefin metathesis catalysts. To our surprise, the developed catalysts facilitated the polymerization of cyclopentadiene (CPD), a feedstock that is easily and commonly obtainable through the steam cracking of naphtha, which has, to the best of our knowledge, not been previously achieved due to its low ring strain and facile dimerization even at low temperatures (below $0\text{ }^{\circ}\text{C}$).



Symposium : **KCS1-4**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 15:00

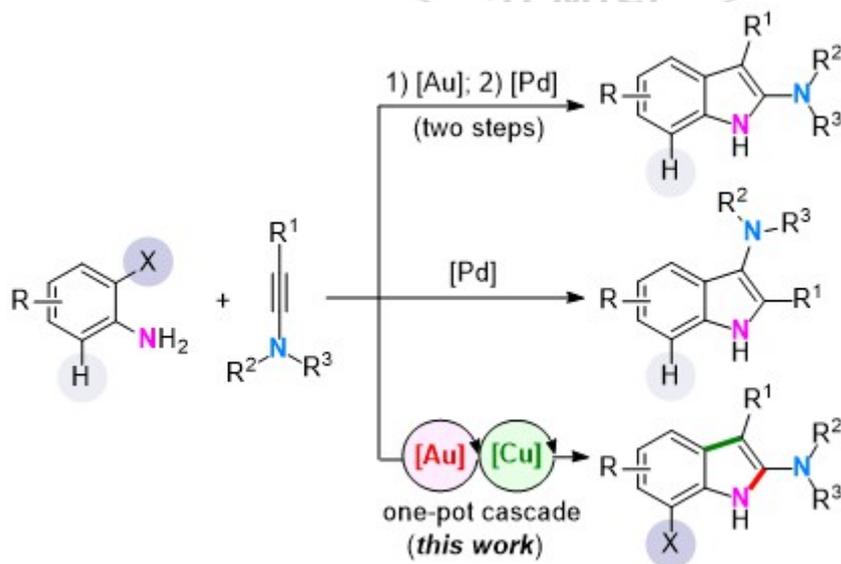
Chair: Cheol-Hong Cheon (Korea University)

Facile One-Pot Synthesis of 2-Aminoindoles from Simple Anilines and Ynamides

So Won Youn

Department of Chemistry, Hanyang University, Korea

Among indoles referred to as “privileged structures,” 2-aminoindoles are important structural motifs found in a wide range of bioactive compounds. While numerous methods for construction of indoles have been developed, synthetic methods to produce 2-aminoindoles have remained limited. In recent years, various synthetic approaches toward 2-aminoindoles using ynamides as versatile building blocks have been developed. Ynamides are useful precursors as a source of either the N1 atom or C2-amino substituent for regioselective formation of the 2-aminoindole scaffold. In this presentation, our recent discovery of a highly efficient and facile one-pot reaction for the synthesis of diversely substituted 2-aminoindoles directly from anilines and ynamides will be described. In this one-pot sequential process, the two metal salts, Au(I) and CuCl₂, operate in two distinct reactions in series.



Symposium : **KCS1-5**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 15:20

Chair: Cheol-Hong Cheon (Korea University)

Direct Chiral NMR analysis and Its Applications to Simultaneous Chiral Analysis.

Hyunwoo Kim

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

Chiral analysis, such as determination of identity, concentration, and the relative ratio of optically active (chiral) molecules, plays an indispensable role in contemporary synthetic, medicinal, and biological chemistry. The most popular technique for chiral analysis is the chromatographic method, which uses chiral stationary phases but in which a usually rather time-consuming step to find the right chiral column is required. However, chromatographic chiral analysis, particularly for unknown chiral compounds, is still a time-consuming and costly procedure, because the analytical ability of each chiral column is highly dependent on the structure and functional moiety of the analytes, and further synthetic efforts are often required. NMR spectroscopy is one of the most convenient and widely-used analytical instruments for the determination of chemical structures. In order to implement in-situ direct chiral analysis using NMR spectroscopy, chiral analytes can be mixed with chiral solvating agents such as coordinatively unsaturated chiral lanthanide or transition metal complexes Brønsted acids/bases, and supramolecular receptors to generate anisotropic signals. In recent years, we introduced charged metal complexes as general and efficient chiral solvating agents working for any time of amines, acids, alcohols, and carbonyl compounds. In addition, we demonstrated that chiral NMR analysis can be expanded to the chiral analysis for one-pot multi-substrate reactions. We believe our new analytical method can be potentially used in the high-throughput chiral analysis.

Symposium : **KCS1-6**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 15:50

Chair: Eun Jin Cho (Chung-Ang University)

Aziridines in Natural Product Synthesis

Hyun-Joon Ha

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Various N-containing natural products alkaloids such as sphingolipids, azasugars, furanomycin, hygrolone, isosolenopsin, microcosames, microgrewiapine, biemamides, etc. were successfully synthesized from aziridine-2-carboxylate based on the functional group transformation of carboxylate and highly ring strained three membered aza-ring heterocycles, aziridines. References, Nikhil, S.; Macha, L.; Ha, H. J. "Stereoselective synthesis of 2,6-disubstituted piperidine alkaloids" *Org. Biomol. Chem.*, 2020, 18, 5493-5512. Ha, H. J. "Editorial: Strained Aza-Heterocycles in Synthesis" *Front. Chem.* 2019, 7, 669. Nikhil, S.; Macha, L.; Ha, H. J. "Total Synthesis and Stereochemical Revision of Biemamides B and D" *Org. Lett.* 2019, 21, 8992-8996.

Symposium : **KCS1-7**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 16:10

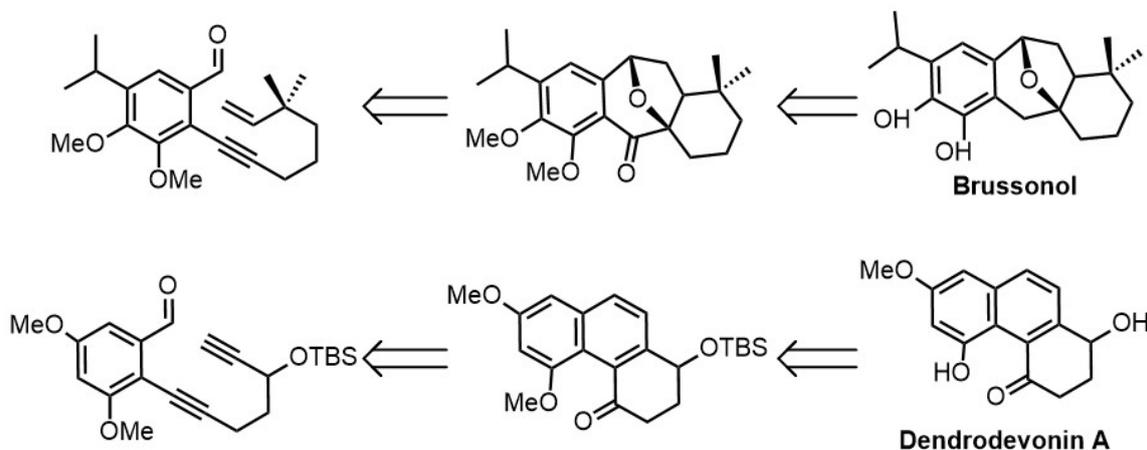
Chair: Eun Jin Cho (Chung-Ang University)

Total Synthesis of [6,m,6] tricyclic natural compounds by gold-catalyzed cyclization

Chang Ho Oh

Department of Chemistry, Hanyang University, Korea

Brussonol was isolated from the root culture of *Salvia broussonetii* and shown to be cytotoxic toward insect and mammalian cell lines. Dendrodevonin A with phenanthrene structure was extracted from the stem of *Dendrobium devonianum*. It has been used in the traditional Chinese medicine “Shihu” and showed cytotoxicity to inhibit the growth of human colon cancer HT-29 cell. Due to the biological activity of brussonol and dendrodevonin A, they are attractive targets for chemical synthesis. Recently, we reported the construction of the [6,m,6] tricyclic skeleton, a key intermediate for synthesizing natural compounds (faveline, komaroviquinone, taxamairin B, rosmaridiphenol, 1-oxomiltirone and arucadiol), through transition-metal catalyzed cyclization (Au, Cu, Pt..). Continuing our interest in cycloaddition reaction by transition metal catalyst, we synthesized [6,6,6] tricyclic compound Dendrodevonin A and [6,7,6] tricyclic compound Brussonol. We synthesized two natural products very quickly and productively through an effective strategy of gold catalyzed cyclization.



Symposium : **KCS1-8**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 16:30

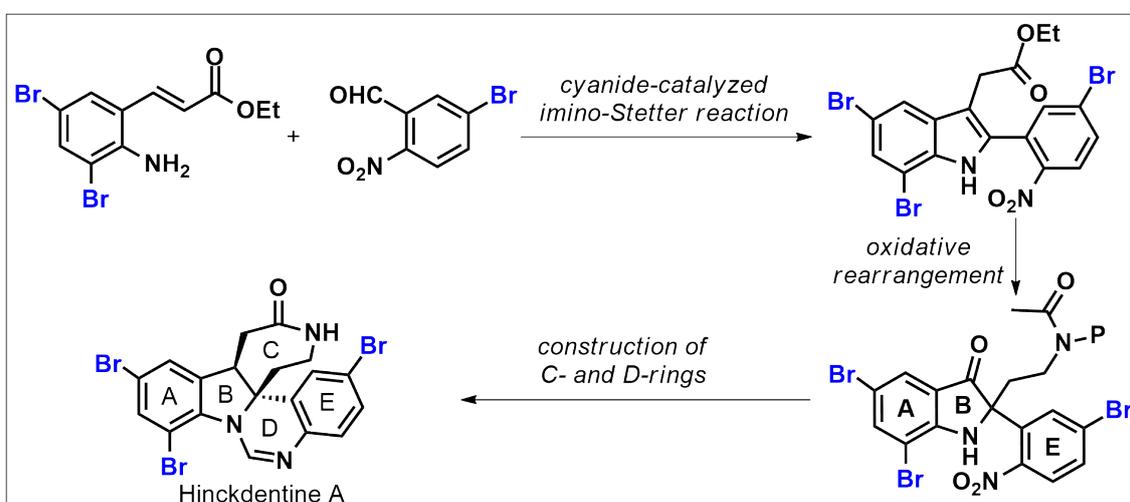
Chair: Eun Jin Cho (Chung-Ang University)

Total Synthesis of Hinckdentine A

Cheol-Hong Cheon

Department of Chemistry, Korea University, Korea

Hinckdentine A, isolated from the marine bryozoan *Hincksinoflustra denticulate* collected from the eastern coast of Tasmania in 1987, possesses a unique structure characterized by a tribrominated indolo[1,2-c]quinazoline core fused to a seven-membered lactam. Because this natural product contains biologically important motifs within its framework, including indoline, azepinone, and quinazoline subunits, it has attracted considerable attention from synthetic and medicinal chemists. In this presentation, the total synthesis of hinckdentine A is described. A cyanide-catalyzed imino-Stetter reaction of the aldimine derived from ethyl 2-amino-3,5-dibromocinnamate and 5-bromo-2-nitrobenzaldehyde, followed by oxidative rearrangement, afforded a 2,2-disubstituted 3-indolinone derivative containing the carbon skeleton and all the functional groups present in the natural product correctly positioned, including three bromine atoms. Subsequent D-ring formation and seven-membered C-ring construction completed the total synthesis of hinckdentine A.



Symposium : **KCS1-9**

[SRC Symposium] New Trends and Developments in Organic Synthesis

Room 304 (Live Streaming) WED 16:50

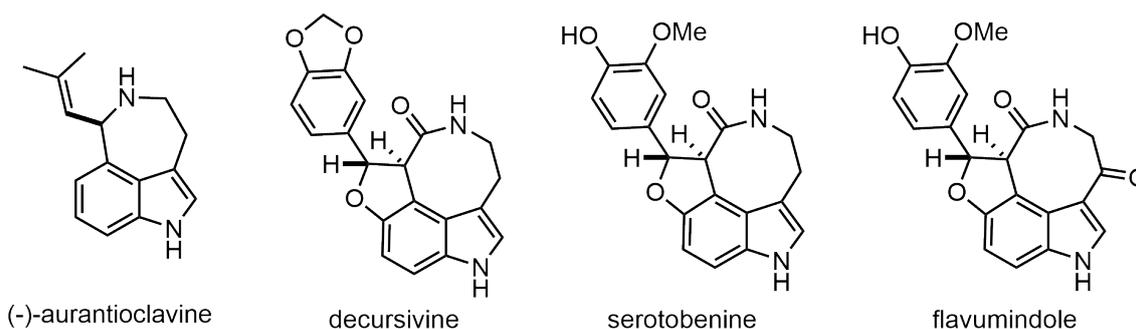
Chair: Eun Jin Cho (Chung-Ang University)

Intramolecular Fischer indole synthesis as novel approach to 3,4-fused tricyclic indole-containing natural alkaloids

Cheon-Gyu Cho

Department of Chemistry, Hanyang University, Korea

We have previously demonstrated that aryl hydrazides are effective surrogates of aryl hydrazines, undergoing various reactions including the Fischer indole synthesis to afford the corresponding indoles, when treated with enolizable aldehydes and ketones in the presence of an acid. Unlike aryl hydrazines, the aryl hydrazides are readily accessed from aryl halides via the Pd(0) or Cu(I)-catalyzed coupling reaction with N-Boc hydrazine. We have also reported that N-Cbz-aryl hydrazide can proceed in a Fischer indolization reaction to give N-Cbz-indole without the elimination of N-Cbz group. Prompted by our recent interest on 3,4-fused tricyclic indole alkaloids, we set out to study the intramolecular Fischer indolization reaction. Recently, we found that the aryl hydrazides with a ketone or aldehyde containing side chains linked to the meta-position of the aromatic ring undergo acid promoted intramolecular Fischer indole synthesis (IMFIS) to generate 3,4-fused tricyclic indoles. The preparative utility of this conceptually new synthetic approach, which does not require cumbersome prefunctionalization of the indole ring, was demonstrated by its application to a concise synthesis of (-)-aurantioclavine. Further applications to various other structurally complex polycyclic indole natural products with 3,4-fused tricyclic indole core including decursivine will be presented.



Symposium : **KCS2-1**

[IBS Symposium] Frontiers in Nanoparticles Chemistry and Their Applications

Room 305 (Live Streaming) WED 14:00

Chair: So-Jung Park (Ewha Womans University)

Chemistry for Nano, and Nano for Medicine & Energy

Taeghwan Hyeon

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

For the last 20 years, I have been focused on the synthesis and medical & enegy applications of uniform-sized nanocrystals and related nanomaterials (Nature Mater. 2004, 3, 891). We reported that uniform 2 nm iron oxide nanoclusters can be successfully used as T1 MRI contrast agent for high-resolution MR angiography of monkeys (Nature Biomed. Eng. 2017, 1, 637). We demonstrated that ceria nanoparticles and ceria–zirconia nanoparticles can work as therapeutic antioxidants to treat various nasty diseases including ischemic stroke, Alzheimer’s disease, sepsis, and Parkinson’s disease (Angew. Chem. Int. Ed. 2012, 51, 11039; ACS Nano, 2016, 10, 2860; Angew. Chem. Int. Ed. 2017, 56, 11399; Angew. Chem. Int. Ed. 2018, 57, 9408; Adv. Mater. 2018, 30, 1807965). CeO₂/Mn₃O₄ nanocrystals possessing surface strains protect tissue-resident stem cells from irradiation-induced ROS damage, significantly increasing the survival rate of the animals (Adv. Mater. 2020, 32, 2001566). We report a highly sensitive and selective K⁺ nanosensor that can quantitatively monitor extracellular K⁺ concentration changes in the brains of freely moving mice experiencing epileptic seizures (Nature Nanotech. 2020, 15, 321).

We present a synthesis of highly durable and active electrocatalysts based on ordered fct-PtFe nanoparticles and FeP nanoparticles coated with N-doped carbon shell (J. Am. Chem. Soc. 2015, 137, 15478; J. Am. Chem. Soc., 2020, 142, 14190; J. Am. Chem. Soc. 2017, 139, 6669). We also report on the design and synthesis of highly active and stable Co-N₄(O) moiety incorporated in nitrogen-doped graphene (Co1-NG(O)) that exhibits a record-high kinetic current density (2.84 mA cm⁻² at 0.65 V vs. RHE) and mass activity (277.3 A g⁻¹ at 0.65 V vs. RHE) with unprecedented stability (>110 h) for electrochemical hydrogen peroxide (H₂O₂) production (Nature Mater. 2020, 19, 436). We report on the design and synthesis of highly active TiO₂ photocatalysts incorporated with site-specific single copper atoms (Cu/TiO₂) that exhibit reversible & cooperative photoactivation process, and enhancement of photocatalytic hydrogen generation activity (Nature Mater. 2019, 18, 620). We synthesized multigrain nanocrystals consisting of Co₃O₄ nanocube cores and Mn₃O₄ shells. At the sharp edges of the Co₃O₄

nanocubes, we observed that tilt boundaries of the Mn_3O_4 grains exist in the form of disclinations, and we obtained a correlation between the defects and the resulting electrocatalytic behavior for the oxygen reduction reaction (Nature 2020, 359, 577).



Symposium : **KCS2-2**

[IBS Symposium] Frontiers in Nanoparticles Chemistry and Their Applications

Room 305 (Live Streaming) WED 14:40

Chair: So-Jung Park (Ewha Womans University)

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

Jinwoo Lee

Department of Chemical and Biomolecular Engineering, KAIST, Korea

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

Symposium : **KCS2-3**

[IBS Symposium] Frontiers in Nanoparticles Chemistry and Their Applications

Room 305 (Live Streaming) WED 15:10

Chair: So-Jung Park (Ewha Womans University)

Crystallization and 3D structures of nanoparticles by in situ TEM

Jungwon Park

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

Molecular or atomistic mechanistic understanding of nucleation, growth, and structural changes of nanoparticles have not achieved enough at the nanoscale or below. It is mainly because of a lack of appropriate analytical methods that can obtain in-situ structural information with a spatial resolution at such small length scale along with sub-msec temporal resolution. The in situ, both in liquid phase and dry state, transmission electron microscopy (TEM) offers an opportunity to directly observe diverse classes of chemical reactions. Here we present application of in situ TEM to study nucleation of metallic nanoparticles. We reveal that the early stage of nanoparticle formation is driven by reversible transition between disordered and ordered phases before crystalline phase is stable above a certain size. It is also frequently observed that different types of non-classical pathway, including two-step nucleation, amorphous-to-crystalline transition, and coalescence of clusters, are heavily involved in different conditions of nanoparticle formation. We also present a new development using liquid phase TEM to investigate 3D atomic structures of nanoparticles directly in the colloidal synthesis batch.

Symposium : **KCS2-4**

[IBS Symposium] Frontiers in Nanoparticles Chemistry and Their Applications

Room 305 (Live Streaming) WED 16:00

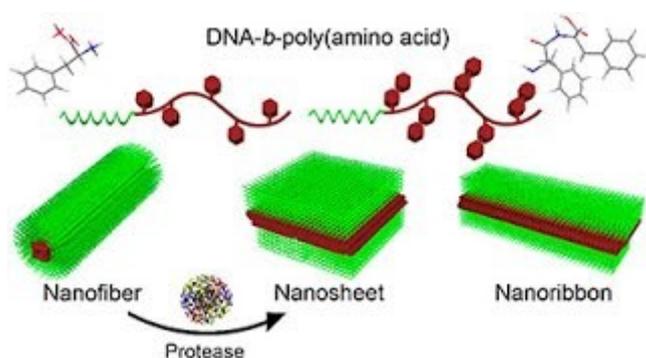
Chair: Jungwon Park (Seoul National University)

Dynamic Nanostructures from Self-Assembly of Functional Polymers and Nanoparticles

So-Jung Park

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

Here, we present two distinct approaches for the fabrication of stimuli-responsive dynamic DNA nanostructures. Firstly, dual-bioactive block copolymers composed of DNA and amino acid-based polymers were synthesized by coupling oligonucleotides to phenylalanine (Phe)-based polymers, which self-assemble into various low-dimensional structures such as nanofibers, ribbons, and sheets through controllable amino-acid interactions. DNA-b-poly(amino acid) assemblies can undergo protease-induced fiber-to-sheet shape transformations, where the morphology change is dictated by the type of enzymes and amino acid sequences. Secondly, we present the fabrication of shape-shifting free-standing films of nanoparticles, based on the programmable DNA-directed self-assembly and the layer-by-layer (LbL) thin film fabrication technique. We demonstrate that the new approach provides a powerful means to generate dynamic nanostructures that can undergo complex and programmable shape transformation.



Symposium : **KCS2-5**

[IBS Symposium] Frontiers in Nanoparticles Chemistry and Their Applications

Room 305 (Live Streaming) WED 16:30

Chair: Jungwon Park (Seoul National University)

Scalable Surface-Enhanced Raman Scattering Nanoprobes for Next-Generation Biomedical Diagnostics

Jwa-Min Nam

Department of Chemistry, Seoul National University, Korea

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



Symposium : **KCS2-6**

[IBS Symposium] Frontiers in Nanoparticles Chemistry and Their Applications

Room 305 (Live Streaming) WED 17:00

Chair: Jungwon Park (Seoul National University)

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.

Symposium : **KCS3-1**

[Tutorial] Mass Spectrometry: Beyond Routine Analysis

Room 304 (Live Streaming) FRI 09:30

Chair: Eunsung Lee (POSTECH)

Mass spectrometry for the structural analysis

Jongcheol Seo

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

Mass spectrometry (MS) has been extremely successful for the molecular identification, and therefore has become one of the most routine identification techniques in the diverse field of research, such as organic/inorganic synthesis, proteomics, metabolomics, and many more. Accurate determination of molecular weight and subsequent chemical stoichiometry, low sample consumption, resistance to the impurities, and several more advantages have made MS the excellent analytical choice for chemical identification. However, it has only limited use for determining structural details of intact molecules and molecular structures, although the development of soft ionization methods such as matrix-assisted laser/desorption ionization (MALDI) and electrospray ionization (ESI) enabled to detect intact macromolecules using MS. Recently since the early 21st century, emerging MS-based experimental techniques has enabled the structural investigation of various molecular species such as molecular self-assemblies, biomolecules, organic-/inorganic clusters, and many more. The representative techniques include hydrogen-deuterium exchange mass spectrometry (HDX-MS), chemical cross-linking, ion mobility-mass spectrometry, gas-phase ion spectroscopy, and several more. These techniques allow us for deducing structural information by identifying solvent-accessible moieties, determining the functional groups in the proximity, revealing molecular collision cross section, and/or obtaining spectroscopic data in addition to mass spectrometric results. In this tutorial, the basic principles of various MS-based structural analysis techniques such as HDX-MS, chemical cross-linking, and IM-MS will be briefly introduced. Their advantages and limitations are discussed as well. In addition, recent applications of such techniques will be presented.

Symposium : **KCS3-2**

[Tutorial] Mass Spectrometry: Beyond Routine Analysis

Room 304 (Live Streaming) FRI 10:30

Chair: Eunsung Lee (POSTECH)

Direct ionization mass spectrometry: imaging and other applications

Sangwon Cha

Department of Chemistry, Dongguk University, Korea

A typical mass spectrometry (MS)-based, complex mixture analysis usually involves intensive chemical extraction and chromatographic separation steps. However, direct sample analysis with minimal sample preparation is sometimes desirable in order to perform high throughput chemical analysis, to obtain chemical information in situ and in real time, or to reveal spatial distribution of analytes of interest directly from a sample surface. For this purpose, direct ionization methods have been developed and actively applied in various scientific fields. In this tutorial, basics, advantages, and limitations of direct ionization methods for MS are going to be briefly discussed. Direct ionization methods to be covered in this tutorial include matrix-assisted laser desorption/ionization (MALDI), desorption electrospray ionization (DESI), direct analysis in real-time (DART), paper spray ionization (PSI), and so on. In addition, various applications of direct ionization MS in chemical science will be introduced. Among these, this tutorial will focus on mass spectrometric imaging, real-time reaction monitoring, microscale chemical synthesis, and raw solid material analysis.

Symposium : **KCS5-1**

[NFEC Symposium] Introduction to “Basic Science Research Capacity Enhancement Project”

Room 304 (Live Streaming) FRI 13:00

Chair: Indong Yeo (KBSI (NFEC))

Introduction of Basic Science Research Capacity Enhancement Project

Indong Yeo

Korea Basic Science Institute(KBSI), Korea

NFEC (The National Research Facilities and Equipment Center) is a government-funded organization that carries out projects such as strategic investment in research facilities and equipment, promotion of co-utilization, and training for professional human resources. NFEC implements deliberation for introduction and transfers equipment and facilities through the ZEUS sharing center and makes a road map. There are some problems about managing facilities and equipment financed by governmental R&D budgets. Since researchers operate and manage equipment individually, it makes duplicated equipment introduction and low co-utilization rate which can lead to investment inefficiency of governmental R&D budget. To solve those problems, we have introduced one of the main project, “Basic Science Research Capacity Enhancement Project” supported by the Ministry of Education. In this project, there are three major tasks, the largest part is ① supporting build-up of “the Core-Facility”. The others are ② introducing research equipment in “Core-Facility” and ③ supporting for co-research revitalization between researchers in “Core-Facility.” Additionally, only designated “Core-Facility” centers can be allowed to participate in ② or ③ tasks.

Specifically, the largest task, building-up “the Core-Facility” is to support funds for the new centers and established centers which need to support the equipment aggregation, integrated operation and also operating personnel analysis services. In addition, we conduct customized consultation with experts at each stage of growth whether or not to keep “the Core-Facility”.

Through the building-up, development and capacity maturity of “the Core-facility”, the site-oriented research ecosystem will be created and the efficient utilization of the governmental R&D budget will be possible. In addition, the co-utilization among researchers will improve the national basic science research capacity.

교육부 기초과학 연구역량 강화사업이란?

교육부에서 2019년부터 신규 사업으로 추진하고 있는 기초과학 연구역량 강화사업은 대학 내 흩어져 잘 활용되지 않는 연구장비를 집적하여 연구분야별로 특화된 공동활용센터인 핵심연구지원센터를 조성 운영하도록 지원하는 사업으로 대학의 연구역량 향상과 효율적인 연구 생태계 조성을 그 목표로 하고 있습니다.



CORE 핵심연구지원센터 Core-Facility

핵심연구지원센터(Core-Facility)란?

핵심연구지원센터(Core-Facility)는 단순 장비 운영, 데이터 산출이 아닌 데이터 해석 등을 통해 전문적 연구지원이 가능한 연구분야별로 특화된 공동활용센터를 의미합니다.

우리나라 핵심연구지원센터(Core-Facility)현황



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연구장비 구축 지원 과제



핵심연구지원센터(Core-Facility)조성 지원 과제를 수행(예정) 중인 핵심연구지원센터의 성장 및 고도화에 꼭 필요한 연구장비 구축을 지원합니다.

지원 기준 1 점(장비)
지원 금액 1~10 억 원 지원

공동연구 활성화 지원 과제



핵심연구지원센터(Core-Facility)조성 지원 과제를 수행(예정) 중인 핵심연구지원센터를 중심으로 한 공동연구가 활성화될 수 있도록 공동연구비를 지원합니다.

지원 기간 3 년
지원 금액 1 억 원 지원(연간)



Symposium : **KCS5-4**

[NFEC Symposium] Introduction to “Basic Science Research Capacity Enhancement Project”

Room 304 (Live Streaming) FRI 13:45

Chair: Indong Yeo (KBSI (NFEC))

Introduction to CNU Chemistry Core-Facility in Chungnam National University

Jeongkwon Kim

Department of Chemistry, Chungnam National University, Korea

The CNU Chemistry Core Facility (Director: Professor Jeongkwon Kim), hosted by the Department of Chemistry, Chungnam National University, was selected as a 'Basic Science Research Capacity Enhancement Project' by the Ministry of Education and Korea Basic Science Institute in 2019. Through this project, research equipment with low utilization will be centralized based on its specialized research field, maximizing its performance. Dedicated personnel will be recruited to successfully operate the research equipment at the Core Facility. The Core Facility is to become a center representing Chungcheong province for chemical substance analysis using chemical analysis equipment belonging to Chungnam National University. Joint use and joint research in the fields of mass spectrometry, separation analysis, material analysis, organic analysis, and structural analysis will be performed through efficient management and operation using various analysis equipment such as microscopes, surface analyzers, spectrophotometers, mass spectrometers, and chromatography instruments. Representative equipment includes environmental scanning electron microscope (E-SEM), X-ray diffractometer, specific surface area measurement device, infrared spectrophotometer (FT-IR), MALDI mass spectrometer (MALDI-MS), liquid chromatography (LC), There are gas chromatography (GC), gas chromatography-mass spectrometry (GC-MS). The researchers belonging to the Department of Chemistry at Chungnam National University who have specialized knowledge about each equipment will provide high-level analysis services. In this presentation, the detailed information of the Core Facility will be provided.

Symposium : **KCS5-5**

[NFEC Symposium] Introduction to “Basic Science Research Capacity Enhancement Project”

Room 304 (Live Streaming) FRI 14:00

Chair: Indong Yeo (KBSI (NFEC))

Introduction to Core-Facility for Bionano Materials in Gachon University

Sang Yun Han

Department of Chemistry, Gachon University, Korea

“Core-Facility for Bionano Materials” is established at Gachon University as a shared-research platform for the emerging research fields of bionano convergence. Its research capacity is particularly aimed to support various efforts to understand bionano materials, e.g. target-oriented nanomedicines, and their behaviors in the biological system. For the purpose, the center integrates the state-of-the-art research instruments in a place and develops the research techniques for individual instruments or by hyphenating them. In the initial stage of establishment, the center presently focuses on (1) characterization of nanomaterials’ properties using HR-TEM, FE-SEM, NTA, and BET, (2) detailed structural analysis of biopolymers using 500MHz NMR, LC-MS, GC-MS, and FT-IR, (3) their behaviors and impacts on the biological systems using confocal microscopy, fluorescence microscopy, and the like. The core-facility further develops the research techniques for the analyses of complex composite materials as well as interfacial chemistry. In addition, using the shared-research platform, the center offers the technical workshops for general audience and the special training programs for advanced researchers. The center also makes significant efforts to create research networks in the related industry and research fields. The core-facility is supported by Basic Science Research Capacity Enhancement Project funded by Ministry of Education via National Research Facilities & Equipment Center of Korea Basic Science Institute.

Symposium : **POLY1-1**

Recent Trends in Early-career Polymer Chemists

Room 403 (Live Streaming) THU 10:40

Chair: Myungeun Seo (KAIST)

Synthesis of P3HT-Coil Block Copolymers by Suzuki-Miyaura Catalyst-Transfer Polycondensation

In-Hwan Lee

Department of Chemistry, Ajou University, Korea

Conjugated block copolymers and their unique self-assembled nanostructures have emerged as valuable materials to enhance the optoelectronic and physical properties of conjugated homopolymers. Owing to their enhanced properties, conjugated block copolymers have found useful applications, for example, as active materials and compatibilizers for organic solar cells, as transporting materials for lithium battery electrodes, and as fluorescent probes for sensing chemicals. To achieve the facile block copolymerization, we developed the coil-first approach using the RuPhos-Pd-catalyzed Suzuki-Miyaura catalyst-transfer polycondensation. The method was successfully produced poly(methyl acrylate)-, poly(methyl methacrylate)-, and poly(ethylene oxide)-block-poly(3-hexylthiophene) with controlled molecular weight, low dispersity, high yield, and easy purification. Further, the combination of the conventional rod-first and newly developed coil-first approaches facilitated the straightforward synthesis of a unique rod-coil-rod triblock copolymer that was limitedly accessible by other methods. We believe this efficient and readily accessible synthetic platform would be highly useful for the preparation of novel conjugated rod-coil block copolymers that can be applied in optoelectronics, battery engineering, and chemical sensing.

Symposium : **POLY1-2**

Recent Trends in Early-career Polymer Chemists

Room 403 (Live Streaming) THU 11:00

Chair: Myungeun Seo (KAIST)

Thermodynamic Synthesis of Ladder-Type Functional Organic/Polymer Materials

Jongbok Lee

Department of Biological & Chemical Engineering, Hongik University, Korea

Conjugated ladder-type macromolecules represent a captivating class of materials on account of their well-defined rigid structures, intriguing syntheses, and promising potential in optoelectronic applications. The ladder-type backbones possess an intrinsically rigid conformation and limit possible torsional disorder. The unique architecture of conjugated ladder-type materials leads to extended π -conjugation length, longer exciton diffusion length, and enhanced stability, compared to conventional conjugated materials. This efficient and versatile synthetic strategy successfully afforded various fused polycyclic heteroarenes, a series of extended ladder-type oligomers, and conjugated ladder polymers with minimum levels of structural defects in excellent yields. Furthermore, RCM demonstrated an excellent ring annulation efficiency with electron deficient acceptor units. This research provides a well-established synthetic strategy to construct a fully conjugated ladder-type material and a fundamental understanding of ladder-type functional organic materials for potential future applications in electronic and optoelectronic devices. This research provides a well-established synthetic strategy to construct a fully conjugated ladder-type material and a fundamental understanding of ladder-type functional organic materials for potential future applications in electronic and optoelectronic devices.



Symposium : **POLY1-3**

Recent Trends in Early-career Polymer Chemists

Room 403 (Live Streaming) THU 11:20

Chair: Myungeun Seo (KAIST)

Responsive, Nanostructured Block Copolymer Particles

Kang Hee Ku

Chemical Engineering and Applied Chemistry, Chungnam National University, Korea

Complex microscale colloids are material platforms for a wide range of sensing scenarios and can be tuned and configured by a variety of chemical and physical phenomena. In particular, the soft boundaries of colloids produce various synergetic effects by exploiting self-assembling polymers. In this talk, I will present the state-of-the-art in programmed design of anisotropically shaped polymer particles driven by phase-separation upon solvent evaporation from interface-engineered emulsions. In particular, two different topics: 1) block copolymer (BCP) particles with reversible shape-changing property activated by wavelength-selective light irradiation, and 2) full-color reflective photonic polymer particles capable of a dynamic color change will be discussed. First, the key to achieving light-responsive shape transitions of BCP particles is the design and synthesis of surfactants containing photo-cleavable groups (i.e., nitrobenzyl esters and coumarin esters) or photo-isomerizable groups (i.e., spiropyran) that modulate the amphiphilicity and interfacial activity of the surfactants in response to light of a specific wavelength. These light-induced changes in surfactant structure modify the surface and wetting properties of BCP particles, affording both shape and morphological transitions of the particles. Next, dendronized brush block copolymers are used to achieve highly ordered axially stacked lamellae with large domain size, allowing a near-perfect photonic multilayer. The photonic ellipsoids are functionalized with magnetic nanoparticles organized into bands on the particle surface to produce real-time on/off coloration by magnetic field-assisted activation.

Symposium : **POLY1-4**

Recent Trends in Early-career Polymer Chemists

Room 403 (Live Streaming) THU 11:40

Chair: Myungeun Seo (KAIST)

Solution self-assembly of copolymer particles : Combined study of theory, simulation and experiment

YongJoo Kim

School of Advanced Materials Engineering, Kookmin University, Korea

Copolymer particles have drawn significant attention as designing functional soft materials and building blocks for colloidal superstructures. Conventional methods for the fabrication of polymeric particles are based on the mechanical deformations which are either expensive and/or improper for large-scale productions. In this study, we suggest the novel methods in controlling size and shape of copolymer particles by changing copolymer architecture in solution self-assembly. By using theory and computer simulation, we designed complex micelles and vesicles. Detailed underlying physics are followed with experimental verification. We believe that our novel strategy will open a new possibility of designing nano-sized soft particles for the functional materials design.

Symposium : **POLY2-1**

Special Symposium by Leading Mid-career Polymer Scientists

Room 403 (Live Streaming) THU 13:00

Chair: Han Young Woo (Korea University)

Molecular Doping toward High Performance Organic Thermoelectric Platform

Bong Gi Kim

Division of Chemical Engineering, Konkuk University, Korea

In order to improve the performance of organic thermoelectric devices, organic semiconductors having high electrical conductivity are essentially required. There are various strategic approaches to enhance the electrical conductivity of organic semiconductors, and we introduce series of studies to secure highly conductive conjugated polymers (CPs) through molecular doping approach, such as blend doping, sequential doping, hybrid doping, and sequential cascade doping. In particular, when adopting indoloindole-based CPs as doping platforms and 2,3,5,6-Tetrafluoro-tetracyanoquinodimethane (F4TCNQ) as a molecular dopant, the resulting electrical conductivity has a significant correlation with the degree of charge transfer (CT) between the CPs and F4TCNQ. In addition, even when the degree of CT is similar, the effectiveness of molecular doping is confirmed to be sensitively affected by the diffusion efficiency of the molecular dopant. Obtained results clearly indicate that structural and morphological considerations are evenly required to obtain highly conductive CPs. Conclusively, through the optimization of dopant diffusion into the indoloindole-based CPs, the doping platform provides excellent thermoelectric properties (26.8 of Seebeck coefficient and 76.1 $\mu\text{W}/\text{mK}^2$ of power factor), including outstanding electrical conductivity (over 600 S/cm).

Symposium : **POLY2-2**

Special Symposium by Leading Mid-career Polymer Scientists

Room 403 (Live Streaming) THU 13:25

Chair: Han Young Woo (Korea University)

Low-Dimensional Single-Cation Formamidinium Lead Halide Perovskites ($\text{FAM}+2\text{PbmBr}_{3m+2}$): From Synthesis to Rewritable Phase-Change Memory Film

Youngjong Kang

Department of Chemistry, Hanyang University, Korea

Synthesis of 2D perovskites often demands long and bulky organic spacer cations, but they hamper optoelectronic properties of the resulting 2D perovskites. Novel low-dimensional single-cation perovskites with a general formula of $\text{FAM}+2\text{PbmBr}_{3m+2}^-$ are prepared by using quenching-assisted solution process, which leads to the wide dimensional control over 1D FA_3PbBr_5 ($m = 1$), 2D $\text{FAM}+2\text{PbmBr}_{3m+2}$ ($m \geq 2$) and 3D FAPbX_3 ($m = \infty$) perovskites simply by changing the composition of precursors. In this case, formamidinium (FA) acts as both A-site cation and spacer cation in $\text{FAM}+2\text{PbmBr}_{3m+2}^-$. Unlike conventional 2D perovskites, $\text{FAM}+2\text{PbmBr}_{3m+2}^-$ perovskites have (110) orientation. PVDF (poly(vinylidene fluoride)) preferentially stabilizes the low-dimensional $\text{FAM}+2\text{PbmBr}_{3m+2}$ phases, and which is utilized to fabricate the stable $\text{FAM}+2\text{PbmBr}_{3m+2}$ -PVDF composite films. The phase transitions from 1D and 2D to 3D are investigated in response to various stimuli including humidity, UV, oxygen and solvents, and which are exploited for rewritable phase-change memory films.

Symposium : **POLY2-3**

Special Symposium by Leading Mid-career Polymer Scientists

Room 403 (Live Streaming) THU 13:50

Chair: Han Young Woo (Korea University)

Advanced Thin Films Fabricated by Coating, Self-Assembling, and Polymerizing Programmed Anisotropic Monomers

Kwang-Un Jeong

Department of Polymer-Nano Science and Tech, Jeonbuk National University, Korea

Anisotropic liquid crystal (LC) networks prepared from reactive mesogens (RM) have numerous advantages in optoelectronic devices especially because of the excellent processability. To fabricate the robust LC thin films with excellent thermal, chemical and mechanical stabilities, the photo-polymerization of anisotropically pre-oriented RMs should be conducted on the optimized conditions. Since the final physical properties of anisotropic LC networks depend on chemical functions and physical intermolecular interactions, the hierarchical superstructures of the programmed RMs with specific chemical functions should be controlled on the different length and time scales before polymerization. The presentation describes the fundamental characteristics and recent research interests of anisotropic LC networks, elastomers and gels fabricated using various programmed RMs.

Symposium : **POLY2-4**

Special Symposium by Leading Mid-career Polymer Scientists

Room 403 (Live Streaming) THU 14:15

Chair: Han Young Woo (Korea University)

Chemical Recycling of Carbon Fiber Reinforced Composites

Munju Goh

Department of Chemical Engineering, Konkuk University, Korea

Carbon-fiber-reinforced plastics (CFRPs) are composite materials weighing only a quarter the weight of steel, but specific strength are 10 times stronger. These strong, stiff, and lightweight materials are an ideal choice for applications where low weight and superior performance are important, for example, as components for aircraft, automobiles, trains, and high-quality consumer products. CFRPs are produced by combining carbon fibers (CFs) with a matrix such as an epoxy (EP) resin. The hardened EP resin forms a three-dimensional cross-linked network structure. Interestingly, this cross-linking between the polymer chains also makes the EP resin infusible and insoluble. In other words, once hardened, an EP resin cannot be remelted to be reshaped; this property distinguishes EP resins from other thermoplastic polymers, which can generally be remelted and reshaped. It should be noted that these properties of the EP resin make it difficult to recycle them. Moreover, recycling challenges are also emerging in CFRPs and other composite materials. It is becoming a substantial problem owing to the environmental pollution caused by the CFRP waste and the reuse of expensive CF resources. In our study, we succeeded in dissolving the epoxy resin within 2h at atmospheric pressure and a reaction temperature of 100 °C are optimal conditions for the depolymerization; this was achieved by using an aqueous solution, which made it possible to recycle these CFRPs. We identified that an initial pH of 12.05 a reaction temperature of 100 °C and are optimal conditions for the depolymerization of CFRP. Moreover, the reclaimed CFs (r-CFs) showed physical properties almost similar to those of virgin CFs (v-CFs). In addition, high value-added products were fabricated by using the carbon fibers (CFs) and resin decomposition products recovered after the decomposition of CFRPs. Thus, the recyclability of CFRPs was maximized to realize minimized the generation of waste.

Symposium : **POLY3-1**

Supramolecular Chemistry of Macromolecules

Room 403 (Live Streaming) THU 14:50

Chair: Kyoung Taek Kim (Seoul National University)

Continuous Printing of Semiconducting Polymer Line Arrays by Meniscus Oscillation Self-Assembly

Jeongjae Wie

Department of Polymer Science and Engineering, Inha University, Korea

Evaporative self-assembly of semiconducting polymers provides a facile preparation of hierarchical micrometer and nanometer-scale features. However, kinetics of solvent evaporation are slow, limiting practical applications toward organic and flexible electronics. In this presentation, we introduce a novel high-throughput and continuous printing technique for semiconducting polymer by a modified doctor blading technique with oscillatory meniscus motion, named meniscus-oscillated self-assembly (MOSA). The oscillatory meniscus motion of the roller generates repetitive stick-slip phenomenon between the roller and polymer solution which can continuously print semiconducting polymer line arrays. The printed lines demonstrate highly defined boundaries and shear force during the printing results in dramatically enhanced crystallinity of polymers. This continuous printing technique can potentially be applied for practical applications in printed electronics.

Symposium : **POLY3-2**

Supramolecular Chemistry of Macromolecules

Room 403 (Live Streaming) THU 15:15

Chair: Kyoung Taek Kim (Seoul National University)

Aggregation-Induced Emission Enhancement of Bis-Arylacylhydrazone-based Supramolecular Assemblies

Changsik Song

Department of Chemistry, Sungkyunkwan University, Korea

Aggregation-induced emission (AIE) phenomena have gained intense interest over the last decades because of its importance in solid-state emission. However, the elucidation of a working mechanism is difficult owing to the limited characterization methods on solid-state molecules, further complicated if dynamic structural changes occur. Here, a series of bis-arylacylhydrazones (BAHs) were synthesized, for which their AIE properties are only turned on by the reversible adsorption of water molecules. We used microcrystal electron diffraction (MicroED) to determine the molecular structures of two BAHs directly from bulk powders (without attempting to grow crystals) prepared in the absence or presence of water adsorption. This study reveals the unambiguous characterization of the dependence of crystal packing on the specific cocrystallization with hydrates. The structural analysis demonstrates that water molecules form strong hydrogen bonds with three neighboring BAH-1, resulting in the almost complete planarization and restriction of the intramolecular rotation of the molecule. MicroED plays an important role in providing a decisive clue for the reversible polymorphism changes induced by the adsorption of water molecules, regulating emissive properties.

Symposium : **POLY3-3**

Supramolecular Chemistry of Macromolecules

Room 403 (Live Streaming) THU 15:40

Chair: Kyoung Taek Kim (Seoul National University)

Intracellular Polymerization-induced Self-Assembly for Supramolecular Approach to Control Cellular Fate

Ja-Hyoung Ryu

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

The polymerization-induced artificial assembly of synthetic building units inside a living cell and the interaction of these assembly with the cellular components have rarely been studied, but are emerging as an intriguing strategy to control cellular fate. We developed intra-mitochondrial polymerization induced self-assembly (Mito-PISA) strategy for constructing polymeric structures by ROS-dissipative system. Targeting mitochondria, the vital organelle for cell survival, has been recognized as an efficient strategy in different therapeutic techniques by disturbing the normal function. Recently, we reported that intra-mitochondrial assembly induced the dysfunction of mitochondria by disrupting the membrane, resulting in the selective apoptosis of cancer cells. In addition, we described a mitochondria-targeting biomineralization system that favorably can induce silicification and consequent apoptosis of various cancer cells. Herein, we report that the in situ disulfide polymerization inside mitochondria is based on both large accumulation of monomers (increased local concentration for polymerization) and high ROS environment (chemical fuel for disulfide reaction). During the polymerization in a mitochondrial reducing environment, the autocatalytic process enables the continuous generation of ROS and the construction of bulky structures for mitochondrial dysfunction. This in-situ polymerization shows great potential for anticancer treatment against various cancer cell lines including drug resistant cancer cell. To the best of our knowledge, this is the first example showing intracellular polymerization to cause mitochondrial dysfunction and these findings can provide a new insight into intracellular polymerization and assembly for the regulation of cellular functions and a therapeutic approach and new targeting platform for the biomedical community.

Symposium : **POLY3-4**

Supramolecular Chemistry of Macromolecules

Room 403 (Live Streaming) THU 16:05

Chair: Kyoung Taek Kim (Seoul National University)

Programming Supramolecular Protein Architectures by Selective Metal-Coordinate Bonding

Woon Ju Song

Department of Chemistry, Seoul National University, Korea

Numerous natural proteins exhibit supramolecular architectures assembled by the multiple copies of protomers. Recently, we reported that selective metal-coordinate bonding programs a protein to create self-assembled supramolecular structures with no necessity for any sequence optimization. Depending on the position of metal-chelate joints, 1-directional, 2-directional, combinatorial, and hierarchical architectures were created. The length and shape of the architectures were also finely tuned by well-defined thermodynamic and kinetic controls. The inherent catalytic activity of the protein was reserved even as in supramolecular structures, suggesting that selective metal-coordinate bonding can be applied for the synthesis and development of functional protein-based materials.

Symposium : **POLY3-5**

Supramolecular Chemistry of Macromolecules

Room 403 (Live Streaming) THU 16:30

Chair: Kyoung Taek Kim (Seoul National University)

In Situ Self-Assembly of Conjugated Polymers

Tae-Lim Choi

Division of Chemistry, Seoul National University, Korea

Conjugated polymers are attractive soft materials that have gained a lot of attentions due to their interesting optoelectronic properties. However, due to their high rigidity and crystallinity, controlling their morphologies are challenging. In this presentation, we will focus on the new strategies for the formation of nanostructures via self-assembly approach. We will introduce a concept of “in situ nano-particllization of conjugated polymers” (INCP) producing various supramolecules directly during the polymerization where no further post-modification is required. Here, we will show three polymerizations, ring-opening metathesis polymerization, cyclopolymerization, and Grignard metathesis polymerization to discuss how various nanostructures are formed in each case. The re-sulting nanostructures are characterized by UV-vis, IR, DLS, AFM, TEM, and optical microscopy to obtain the detailed structural information. Furthermore, we will introduce very simple one-shot polymerization to achieve INCP and this greatly simplifies the process getting to nanostructures. Lastly, we will finish this talk by combining the concept of crystallization-driven self-assembly in order to control their sizes.

Symposium : **INORI-2**

Past, Present, and Future of Energy and Environmental Inorganic Chemistry in Korea

Room 402 (Live Streaming) THU 10:10

Chair: Jungwon Park (Seoul National University)

2D Inorganic Nanosheet-Based Hybrids for Renewable Energy Applications

Seong-Ju Hwang

Department of Materials Science and Engineering, Yonsei University, Korea

The monolayered 2D nanosheets of layered inorganic solids (layered metal oxides, layered double hydroxides, layered metal chalcogenides, layered metal carbides, and graphene) attract intense research interest because of their versatile roles in multifunctional nanohybrids applicable for renewable energy technologies. The monolayered 2D nanosheets of inorganic solids can be synthesized by soft-chemical exfoliation reaction of the pristine layered materials. A great diversity in the chemical compositions, crystal structures, and defect structures of inorganic nanosheets provides this class of materials with a wide spectrum of physical properties and functionalities. The inorganic nanosheets can be used as powerful building blocks for exploring high performance hybrid electrodes and catalysts. These materials can play a role as active components, additives, and substrates for improving the energy performance of hybridized species. In this talk, several practical examples of 2D monolayered nanosheet-based electrodes and photocatalysts/electrocatalysts for renewable energy storage and generation will be presented together with the discussion about the relationship between chemical bonding nature and functionalities.

Symposium : **INOR1-3**

Past, Present, and Future of Energy and Environmental Inorganic Chemistry in Korea

Room 402 (Live Streaming) THU 10:30

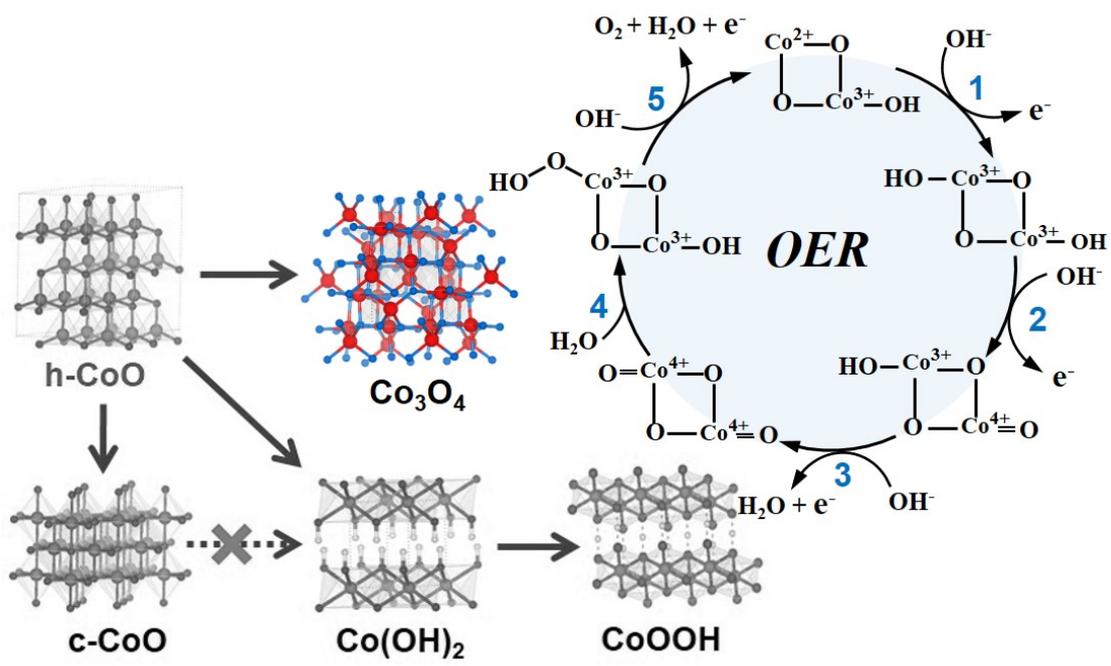
Chair: Jungwon Park (Seoul National University)

A New Synthetic Approach to Cobalt Oxides: Designed Phase Transformation for Electrochemical Water Splitting

Ki min Nam

Department of Chemistry, Pusan National University, Korea

The structural phase transformations of non-native hexagonal CoO (h-CoO) into various other cobalt oxides, such as cubic rock-salt CoO, spinel Co₃O₄, trigonal Co(OH)₂, and trigonal CoOOH, were examined by controlling the reaction conditions. The transformation pathway of h-CoO for each cobalt oxide was fully elucidated. The prepared cobalt oxides were studied as catalysts for oxygen evolution reaction (OER) to clarify the structure-activity relationship. Among the cobalt oxide materials, spinel Co₃O₄ showed the best catalytic activity. Moreover, spinel Co₃O₄ was deposited directly via the oxidative phase transformation of h-CoO particles on a conductive substrate without additional coating processes. The efficient chemical adhesion of spinel Co₃O₄ via phase transformation indicated fast oxidation of Co³⁺ to Co⁴⁺, which resulted in improved OER activity.



Symposium : **INORI-4**

Past, Present, and Future of Energy and Environmental Inorganic Chemistry in Korea

Room 402 (Live Streaming) THU 10:50

Chair: Jinho Chang (Hanyang University)

Bi- and Mono-nuclear Metal Complexes for HX-splitting and their Applications

SeungJun Hwang

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

We have developed bimetallic catalysts that mediate the energy-storing photochemical splitting of HCl to H₂ and Cl₂. We have demonstrated HCl-splitting photocatalysis with two closely related bimetallic Rh₂ catalysts. The critical chemical step with either catalyst is the energy-storing photoelimination of Cl₂. Using transient absorption spectroscopy, a time-resolved photochemical experiment, halogen elimination chemistry from each of these catalysts was shown to proceed through a common reaction intermediate. We have carried out low-temperature steady-state photocrystallography experiments that have established that chloride-bridged intermediates are the structural lynchpins of halogen elimination reactions during catalysis. Our research efforts has been transitioning from second- and third-row transition metal complexes to inexpensive and earth-abundant first-row transition elements for photochemical HX splitting platforms and applying them to bond functionalization. Similar to transient metal-oxos, fleeting halogen radical intermediates are implicated in a host of C–H bond activations. Thus, we develop a series isosteric and isoelectronic pyridine diimine scaffolds in order to study stereo–electronic effects governing photohalogen elimination from cationic Fe(III)Cl₂ centers. A major focus of this work is to move away from the isolation of reactive intermediates and instead generate these transient unstable intermediates in a crystalline lattice and study them using photocrystallography. We have been able to structurally observe the first instance of a C–H bond activation in the solid state. Additionally, we were able to confirm the solid-state assignment of C–H activation by a photoeliminated halogen radical through a combination of EPR, Mass, NMR, and TA studies.

Symposium : **INORI-5**

Past, Present, and Future of Energy and Environmental Inorganic Chemistry in Korea

Room 402 (Live Streaming) THU 11:10

Chair: Jinho Chang (Hanyang University)

From Dye-sensitized Solar Cell to Perovskite Solar Cell

Nam-Gyu Park

School of Chemical Engineering, Sungkyunkwan University, Korea

Since the seminal report on dye-sensitized solar cell (DSSC) in 1991, demands on low-cost photovoltaic technologies start to increase. The initial power conversion efficiency (PCE) of DSSC was about 7%, which was improved to about 10% in about 7 years. The PCE of DSSC was however much lower than the conventional Si solar cell, which suffers from finding suitable applications except for colorful window BIPV. Research activities on DSSC in Korea began since 2000. Korea Organic Solar Cell Society, proposed by Prof. Sung-Hwan Han, was organized in 2001, which contributed significantly to research and development of DSSC. Despite great efforts to improve efficiency of DSSC, its PCE seems to be limited to about 12%. Thus a new technology for higher PCE was required. In 2012, a new technology based on halide perovskite showing a PCE of 9.7% with 500 h-stability was reported by Park's research team, which is called perovskite solar cell (PSC). Since then, PCE of PSC was sweetly increased to over 25% in less than 10 years due to superb optoelectronic properties of halide perovskite. PSC's efficiency surpassed the conventional thin film technologies of CIGS and CdTe and is almost comparable to the PCE of single crystalline Si solar cell. Thus PSC is regarded as a most promising PV technology. In this talk, a brief history of PSC will be introduced and research progress and perspective of PSC will be also discussed.

Symposium : **INORI-6**

Past, Present, and Future of Energy and Environmental Inorganic Chemistry in Korea

Room 402 (Live Streaming) THU 11:30

Chair: Jinho Chang (Hanyang University)

Optimization of energy and environment by inorganic and catalytic chemistry in Korea

Sung-Hwan Han

Department of Chemistry, Hanyang University, Korea

Energy and Environment is two sides of the same coin. They should be well-balanced, if not, there would be a large distortion on one side. There is no satisfaction. Production/consumption of energy and improvement of environment at the same time is the violation of the 2nd thermodynamic law. Therefore there needs to be a compromise between them for the present as well as the future of our descendants. The energy production is related to the reduction chemistry like photosynthesis, and the consumption is to oxidation. The reduction/oxidation reaction is based on the electron transfer, and the understanding of its inorganic chemistry is necessary. Our country is isolated like a single reactor of energy and environment. If we can arrange the energy sources effectively, such as solar, atomic power, fossil fuel, and regenerative energies with the help of inorganic chemistry and catalytic chemistry, we may be able to optimize the energy and environment for the present and future.

Symposium : **INOR2-1**

Past, Present and Future of Coordination Chemistry in Korea

Room 402 (Live Streaming) THU 13:00

Chair: Eunji Lee (Gangneung-Wonju National University)

Preparation and Structural Characterization of Metal Complexes of 1,10-dithia-18-crown-6

In-Hyeok Park

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

A range of divalent metal complexes (**1-12**) of 1,10-dithia-18-crown-6 (**L**) were synthesized in benzonitrile and structurally characterized.[1] In particular cases (Cd and Hg), the anion effect on the resulting structures was investigated. **L** reacts with CdX_2 ($X = \text{ClO}_4$ and NO_3) to yield respective $[\text{Cd}(\text{L})(\text{ClO}_4)_2]$ (**5**) and $[\text{Cd}(\text{L})(\text{NO}_3)_2][\text{Cd}(\text{NO}_3)_4]$ (**6**). In perchlorato-complex **5**, all six donors in **L** participate in the coordination sphere, in which the eight-coordinated 'tight and bent' conformation is completed by two perchlorate ions, adopting a dicapped trigonal prism geometry. Interestingly, the nitratocomplex **6** features three separated units of formula $[\text{Cd}(\text{L})(\text{NO}_3)_2][\text{Cd}(\text{NO}_3)_4]$: two macrocyclic complex cation units and one cadmium quadru-nitrato complex anion unit. In the reaction with HgX_2 ($X = \text{ClO}_4$ and NO_3), **L** afforded an unusual triple-decker type dinuclear complex $[\text{Hg}_2(\text{L})_3](\text{ClO}_4)_4$ (**7**) with 3:2 (**L**:**M**) stoichiometry and a 1:1 complex $[\text{Hg}(\text{L})(\text{NO}_3)_2] \cdot 2\text{H}_2\text{O}$ (**8**) with eight-coordinate, adopting a distorted hexagonal bipyramid geometry.

Reference

[1] I.-H. Park, K.-M. Park, S. S. Lee, *Dalton Trans.* **2010**, 39, 9696-9704.

Symposium : **INOR2-2**

Past, Present and Future of Coordination Chemistry in Korea

Room 402 (Live Streaming) THU 13:10

Chair: Eunji Lee (Gangneung-Wonju National University)

From Silver Complexes with Acyclic Ligands To Chiral Silver Ion-Coordinated Supramolecular Polymers

Jong Hwa Jung

Department of Chemistry, Gyeongsang National University, Korea

Helical metallocupramolecular nanostructures composed of metal-ligand complexes have rapidly developed into one of the most successful and versatile strategies in supramolecular chemistry, because they play essential roles in the formation of superstructures such as the coiled-coil helix bundle proteins, and DNA superhelices, which lead to their potential applications for recognition, catalysis, and ion transport. Thus, I will present a unique dynamic morphology transformation of Ag(I)-coordinated supramolecular nanostructure accompanying the conversion of complex structures in aqueous solution. In the presence of AgNO₃ (1.0 equiv.), the achiral bipyridine-based ligand, possessing hydrazine and glycine moieties, preferentially generated a 1D-needle-like structure (nanostructure I) as a metastable product. Nanostructure I was then transformed into nanostructure II, which was composed of the 1G₃Ag₂(NO₃)₂ complex (1G:Ag⁺ = 3:2) as the thermodynamically stable product. This nanostructure exhibited a 1D-helical tubular structure with a uniform diameter via a 2D-ribbon as an intermedator, which led to the generation of a CD signal with right-handed (P-type) helicity. This study may open up new avenues to the understanding of a dynamic morphology transformation process in biological systems.

Symposium : **INOR2-3**

Past, Present and Future of Coordination Chemistry in Korea

Room 402 (Live Streaming) THU 13:30

Chair: Eunji Lee (Gangneung-Wonju National University)

Covalent Modification of MOF-74

Myoung Soo Lah

Department of Chemistry, Ulsan National Institute of Science and Technology, 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 aminosalicyclic 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(DOBPD), an expanded analog of MOF-74.

Symposium : INOR2-4

Past, Present and Future of Coordination Chemistry in Korea

Room 402 (Live Streaming) THU 13:50

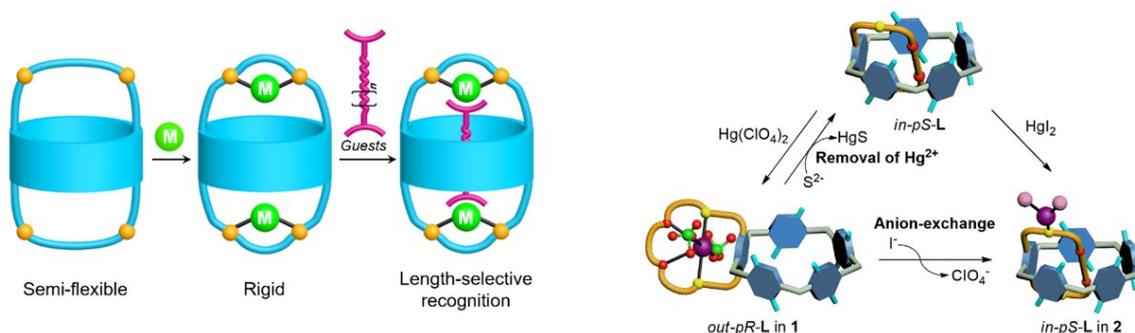
Chair: In-Hyeok Park (Chungnam National University)

Pillar[5]-thiacrowns Exhibiting Guest Molecular Recognition and Metal Ion-Triggered Planar Chiral Inversion

Eunji Lee

Department of Chemistry, Gangneung-Wonju National University, Korea

Pillar[5]-thiacrowns that recognize specific guest molecules via the metal-driven adaptation are reported. In the assembly reactions of pillar[5]-bisthiacrown (**L**) with a series of dicyanoalkanes $[\text{CN}(\text{CH}_2)_n\text{CN}]$, $n = 2-6$ as organic guests, **L** shows a selective affinity to dicyanoethane $[\text{CN}(\text{CH}_2)_2\text{CN}]$, shortly **C2** in the presence of metal ions. The observed results suggest that the selective binding is strongly associated with the metal coordination-induced conformational change. A *pseudo*[1]catenane-type pillar[5]thiacrown (*rac*-**L**) was synthesized and the two enantiomers (*in-pS*-**L** and *in-pR*-**L**) were resolved. Interestingly, the *in-pS*-**L** recognizes Hg^{2+} to trigger the chiral inversion to *out-pR*-**L** in the presence of ClO_4^- or NO_3^- among the anions used. In the mercury(II) perchlorate complex solution, anion-exchange from ClO_4^- to I^- or removal of Hg^{2+} by addition of S^{2-} makes the system reversible. In addition, a one-pot reaction of thiopyridyl-armed pillar[5]arene with silver(I) trifluoroacetate in the presence of the linear dinitrile guest molecule **C8**, $[\text{CN}(\text{CH}_2)_8\text{CN}]$, afforded a two-dimensional (2D) poly-pseudo-rotaxane.



Symposium : **INOR2-5**

Past, Present and Future of Coordination Chemistry in Korea

Room 402 (Live Streaming) THU 14:00

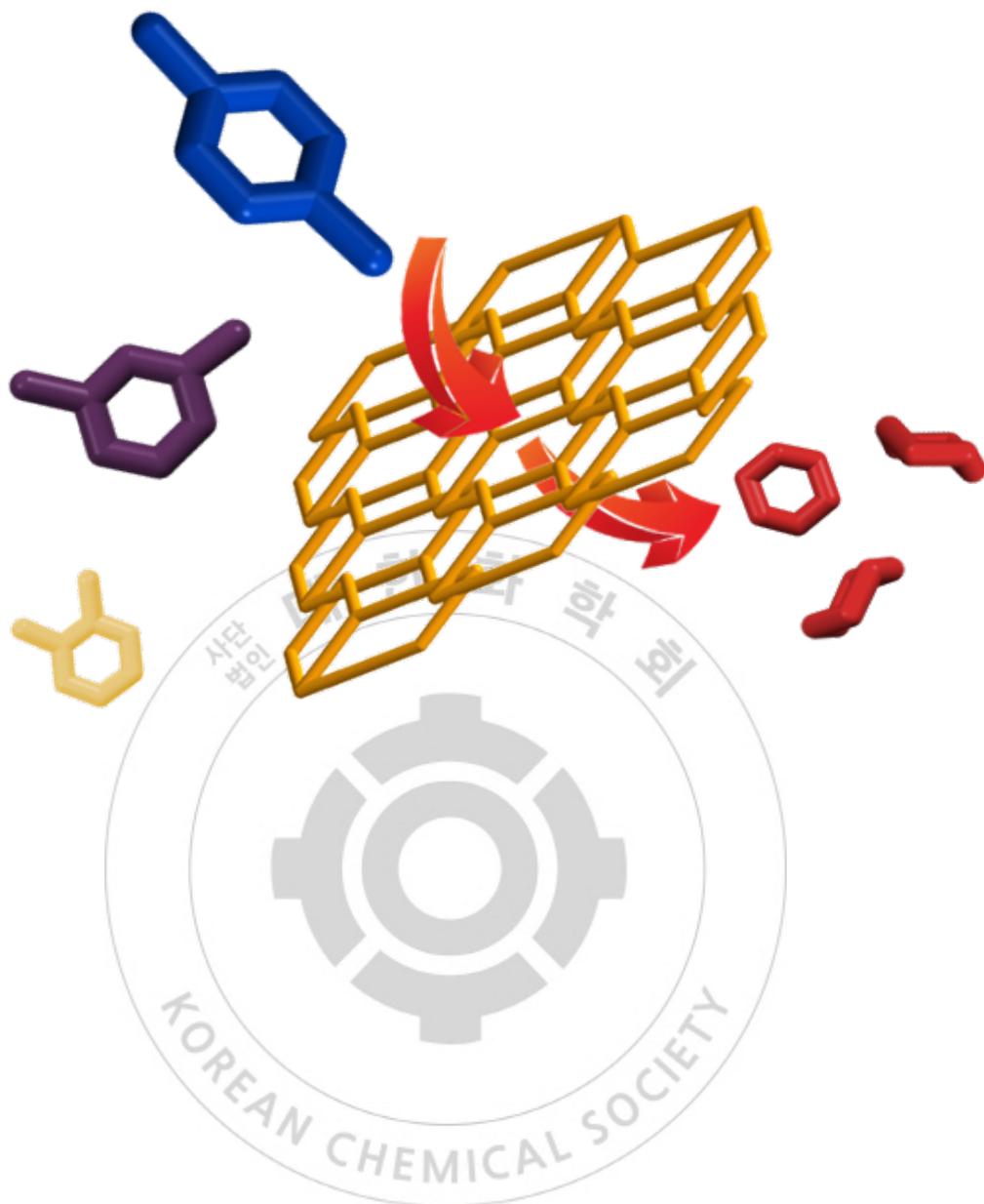
Chair: In-Hyeok Park (Chungnam National University)

Pseudo-2D Porous Networks via Interpenetration of 1D Coordination Polymers: Adsorption and Separation of Xylene Isomers.

Ok-Sang Jung

Department of Chemistry, Pusan National University, Korea

Self-assembly of AgX ($X^- = PF_6^-$, ClO_4^-) with a new C_3 -symmetric tridentate N-donor ligand gives rise to unusual pseudo-2D porous networks with open channels via the interpenetration of 1D zigzag ladders. The open-channel networks selectively adsorb only *m*-xylene from the mixture of *o*- and *m*-xylene, *o*-xylene thus acting as a channel-entrance stopper at room temperature. This system exemplifies unprecedented separation of *o*- and *m*-xylene. The open-channel crystal significantly also shows both temperature and mixture effects on adsorption of *o*-, *m*-, and *p*-xylene isomers in a single-crystal-to-single-crystal (SCSC) mode. *o*-xylene is not adsorbed into the channel at 5°C, but is inserted into the channel at room temperature. Especially, the 1 : 1 mixture of *o*- and *o*-xylene was adsorbed into the channel in the 1 : 1 mole ratio via intermolecular weak interactions at 5°C.



Symposium : **INOR2-6**

Past, Present and Future of Coordination Chemistry in Korea

Room 402 (Live Streaming) THU 14:20

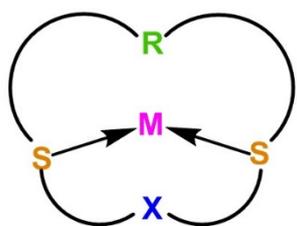
Chair: In-Hyeok Park (Chungnam National University)

My research works on metallosupramolecular chemistry at Gyeongsang National University

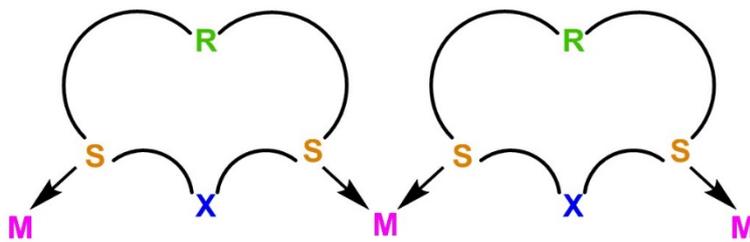
Shim Sung Lee

Department of Chemistry, Gyeongsang National University, Korea

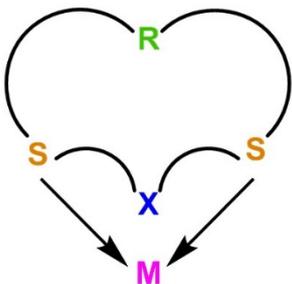
Macrocyclic coordination chemistry has been a center of supramolecular science for last five decades. Due to not only the personal enthusiasm but also the surge in merging to the nanoscience, the title area became a long-lasting research topic during my staying at Gyeongsang National University since 1984. The original intent of this presentation is to serve as a concise introduction of our group's works on the metallosupramolecular chemistry of (thia)crowns and their extended derivatives in the fields of calixarenes and pillararenes. From these building blocks, assembly of large single supramolecules and low to high dimensional coordinative networks including polycatenanes and polyrotaxanes in either endo- or exocyclic mode (*see below*) have been our great interests. The exo-coordination approach toward the coordinative networking is opening up a new supramolecular coordination chemistry by bridging the macrocyclic coordination chemistry and metal-organic frameworks (MOFs). In particular, structural transformation of these materials via an SCSC manner by external stimuli including heat, light, and anion-exchange have been our hot issues. In some cases, metal ion-induced and anion-controlled supramolecular system provides not only the exciting fundamental properties but also their applications. For example, structure-property relation acts as sensors and photo-switches. Owing to lack of time, only some outlines or key points are mentioned. Finally, I would like to thank all the collaborators and group members for their excellent contributions, and the organizing committee of this symposium.



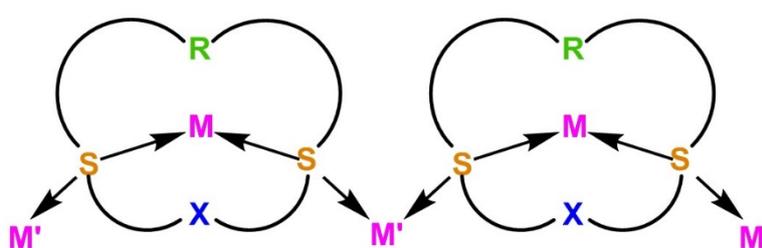
(a) Endocyclic Coordination
(Non-Bridging)



(b) Exocyclic Coordination
(Bridging)



(c) Exocyclic Coordination
(Non-Bridging)



(d) Endo/Exocyclic Coordination
(Bridging)



Symposium : **INOR3-1**

From fundamentals to applications: MOF Chemistry

Room 402 (Live Streaming) THU 15:00

Chair: Seung Jun Hwang (POSTECH)

Plasmonic nanoparticles with nanogap for ultrasensitive biosensors

Jeong-Wook Oh

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Plasmonic nanoparticles have characteristic optical properties such as absorption and scattering in the visible range. When the nanogap is formed inside plasmonic nanoparticles (i.e., *intra*-nanogap) or between nanoparticles (i.e., *inter*-nanogap), the peak wavelengths or the intensities are significantly changed. We developed ultrasensitive optical biosensors by manipulating the nanogap of plasmonic nanoparticles. ~1-nm plasmonic *intra*-nanogap nanoparticles produce a highly enhanced, uniform, and reliable surface-enhanced Raman scattering (SERS) signal. The *intra*-nanogap between core and shell can be controlled by the DNAs modified on core nanoparticles. Not only the *intra*-nanogap but also the exterior surface roughness of nanogap nanoparticles can enhance the SERS signals, enabling the application to biosensors and bioimaging. Also, we developed an *in-situ* DNA hybridization monitoring platform using dynamic plasmonic nanodimers with *inter*-nanogap. This platform is based on tracing dynamic dark-field scattering signals of plasmonic nanodimers corresponding to the association and dissociation events of a single DNA duplex on a supported lipid bilayer pattern. Our results can provide valuable guidelines for developing new plasmonic nanogap structures and their biomedical applications.

Symposium : **INOR3-2**

From fundamentals to applications: MOF Chemistry

Room 402 (Live Streaming) THU 15:20

Chair: Jinhee Park (DGIST)

Twisting of zeolitic imidazolate frameworks into zeolitic imidazolate sulfate frameworks

Jaheon Kim

Department of Chemistry, Soongsil University, Korea

Zeolitic imidazolate frameworks (ZIFs) composed of metal ions and bridging imidazolates are useful for gas adsorption, gas separation, and catalysis. We have developed new three-dimensional frameworks, zeolitic imidazolate sulfate frameworks (ZISFs). They mimic ZIFs by connecting zinc ions with both imidazolate and sulfate bridging ligands. The challenge to the synthesis of ZISFs was to incorporate both organic and inorganic linkers in the frameworks. When 2-methylimidazole (HmIm) was reacted with zinc sulfate, a discrete complex formulated as $(\text{Me}_2\text{NH}_2)_2[\text{Zn}(\text{HmIm})(\text{SO}_4)_2]$ was obtained. A similar compound was obtained for 2-ethylimidazole (HeIm), where imidazole molecules are not deprotonated. A two-dimensional corrugated framework was produced when benzimidazole (HBIm) was used instead of those imidazoles. The phenylene rings of BIm linkers protrude on each side of the layer, leading to a stacking structure. When 2-nitroimidazole (HnIm) was reacted with zinc sulfate, we could obtain a three-dimensional ZISF with GIS topology. In the ZISF-1, characteristic four-membered rings (4MRs) with four Zn vertices and four imidazolate edges, a structural unit commonly found in ZIFs, are linked through sulfate ions to give spaces filled with dimethylammonium ions. Alternatively, we employed 2-mercaptobenzimidazole (HBIm-SH) as a sulfate source, and 2-nitroimidazole (HnIm) was reacted with zinc nitrate to give a pillared three-dimensional ZISF-2. In ZISF-2, 6MRs composed of six Zn ions and six nIm linkers connected further with sulfate ions to form flat layers. Then, these layers are linked by zinc ions located between the layers to create a 3D network. Solvent molecules occluded between the layers in ZISF-2 could be removed to afford a void space, which has been verified by various gas adsorption measurements using N_2 , H_2 , CO_2 , and CH_4 gases. We will present the syntheses, crystal structures, and gas adsorption properties of the compounds mentioned above. We will also show other results about ZIFs that are not routinely synthesized. We believe our achievements will widen a research area concerned with porous and functional ZIFs. This

work was supported by the National Research Foundation of Korea (NRF-2016R1A5A1009405 and NRF-2020R1A2C1004717).



Symposium : **INOR3-3**

From fundamentals to applications: MOF Chemistry

Room 402 (Live Streaming) THU 15:40

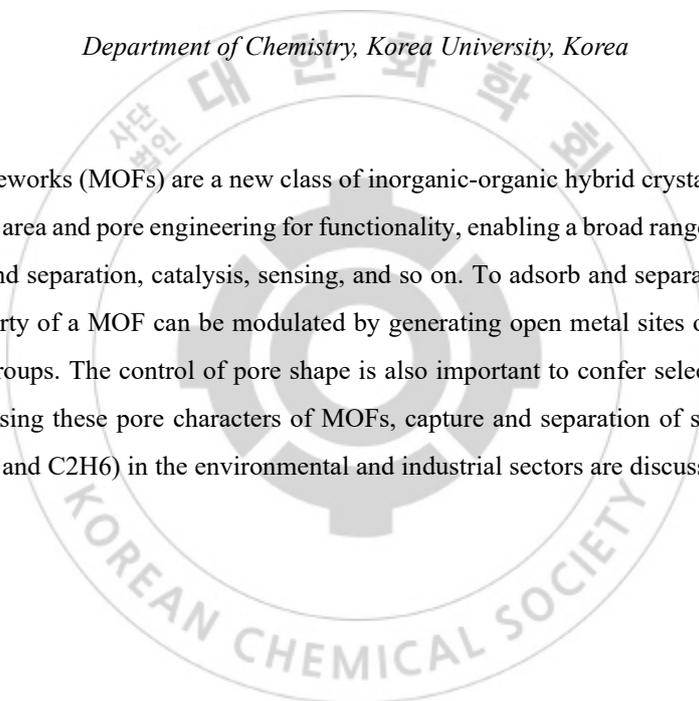
Chair: Jinhee Park (DGIST)

MOF-based adsorbents for capture and separation of specific gases

Chang Seop Hong

Department of Chemistry, Korea University, Korea

Metal-organic frameworks (MOFs) are a new class of inorganic-organic hybrid crystalline materials. They feature high surface area and pore engineering for functionality, enabling a broad range of applications such as gas adsorption and separation, catalysis, sensing, and so on. To adsorb and separate specific gases, the pore size and property of a MOF can be modulated by generating open metal sites or grafting them with proper functional groups. The control of pore shape is also important to confer selective interaction with target molecules. Using these pore characters of MOFs, capture and separation of some important gases (CO₂, NH₃, C₂H₄, and C₂H₆) in the environmental and industrial sectors are discussed in this talk.



Symposium : **INOR3-4**

From fundamentals to applications: MOF Chemistry

Room 402 (Live Streaming) THU 16:00

Chair: Jinhee Park (DGIST)

Specific Isotope-Responsive Breathing Transition in Flexible Metal-Organic Frameworks

Hyunchul Oh

Department of Energy Engineering, Gyeongsang National University (GNU), Korea

A MIL-53(Al), the most well-known flexible metal–organic framework (MOF), leads to (single-step) dynamic changes for hydrogen as closed pore (cp) transitions to open pore (op), also called ‘breathing’ phenomenon. During the flexible and reversible transition by such breathing phenomenon, the pore apertures are continuously adjusted, thus providing the tremendous opportunity to separate mixtures of hydrogen isotope that require precise pore tuning. Recently, we have reported a strategy for effectively separating hydrogen isotopes through this single-step breathing of MIL-53(Al) (JACS, 139, 17743, 2017). Herein, a unique isotope-responsive breathing transition of the flexible metal-organic framework (MOF), MIL-53(Al), which can selectively recognize and respond to only D₂ molecules through a “secondary breathing transition”, is newly reported. This unique isotope selective 2nd breathing transition of MIL-53 are carefully studied through the H₂ and D₂ sorption analysis at various temperatures and in-situ neutron diffraction measurements. To the best of our knowledge, such a flexible system capable of recognizing and responding only to specific isotope molecules has not been reported previously, and it is referred to as the isotope-responsive breathing. Moreover, a large amount of pure D₂ (7.9 mmol g⁻¹) adsorbed in 2nd breathing can be easily recovered by simply decreasing pressure from 850 mbar to 40 mbar, which shows the tremendous potential of flexible MOF as an energy efficient D₂ separation system by combining pressure swing or temperature swing cycles.

Symposium : **INOR3-5**

From fundamentals to applications: MOF Chemistry

Room 402 (Live Streaming) THU 16:20

Chair: Minyoung Yoon (Kyungpook National University)

Exploring the Role of Metal Node Coordination and Modification of Metal-Organic Frameworks and Their Applications

Young Kyu Hwang

Chemical & Process Technology Division, Korea Research Institute of Chemical Technology, Korea

Catalytic transfer hydrogenation (CTH) reaction is considered as a potential route for upgrading bio-based carbonyls to their corresponding alcohols. Herein, a series of Zr-based metal organic frameworks (Zr-MOFs) containing various types of metal node to ligand coordination were synthesized and tested for CTH of furfural (FUR) to furfuryl alcohol (FOL). It was found that metal node coordination plays a more important role than porosity in Zr-MOFs. MOF-808 (synthesized using a scaled-up approach to achieve a higher batch yield), with the lowest metal node to ligand coordination (coordination number = 6), was found to be the most active catalyst among the various tested Zr-MOFs. Furthermore, M-MOF-808, modified by simple methanol activation (M), outperformed the pristine MOF-808 in CTH of FUR to FOL even at 30 °C in the presence of 2-propanol (IPA) as the hydrogen source. The simple modification of the metal node in Zr-MOF changed the acid-base properties of MOF-808 surface through the development of coordinatively unsaturated sites (CUS), hydroxyl and methoxy groups in the framework of the Zr-MOF, which probably helps to facilitate the adsorption of FUR and IPA onto the metal node surfaces of the catalyst. To evaluate the versatility of methanol activation in CTH, further substrates, including other types of biomass and representative carbonyl compounds over M-MOF-808, were tested. To demonstrate heterogeneous catalysis, the catalyst was recycled for five consecutive cycles, with little loss after the first cycle, and was fully characterized to observe any changes in its structure. Mechanistic insights were provided by isotopically labeled isopropanol-d8 experiments, indicating FUR reduction through transfer hydrogenation. Finally, I will present the reaction mechanism for CTH of FUR to FOL was proposed in detail using density functional theory (DFT) calculations over metal node modified model systems of 6-connected Zr-MOF. In addition, I will briefly present the recent results on unique design of superior metal-organic framework for removal of toxic chemicals in humid environment via direct functionalization of the metal nodes in MOF-808 (Zr).

Symposium : **INOR3-6**

From fundamentals to applications: MOF Chemistry

Room 402 (Live Streaming) THU 16:40

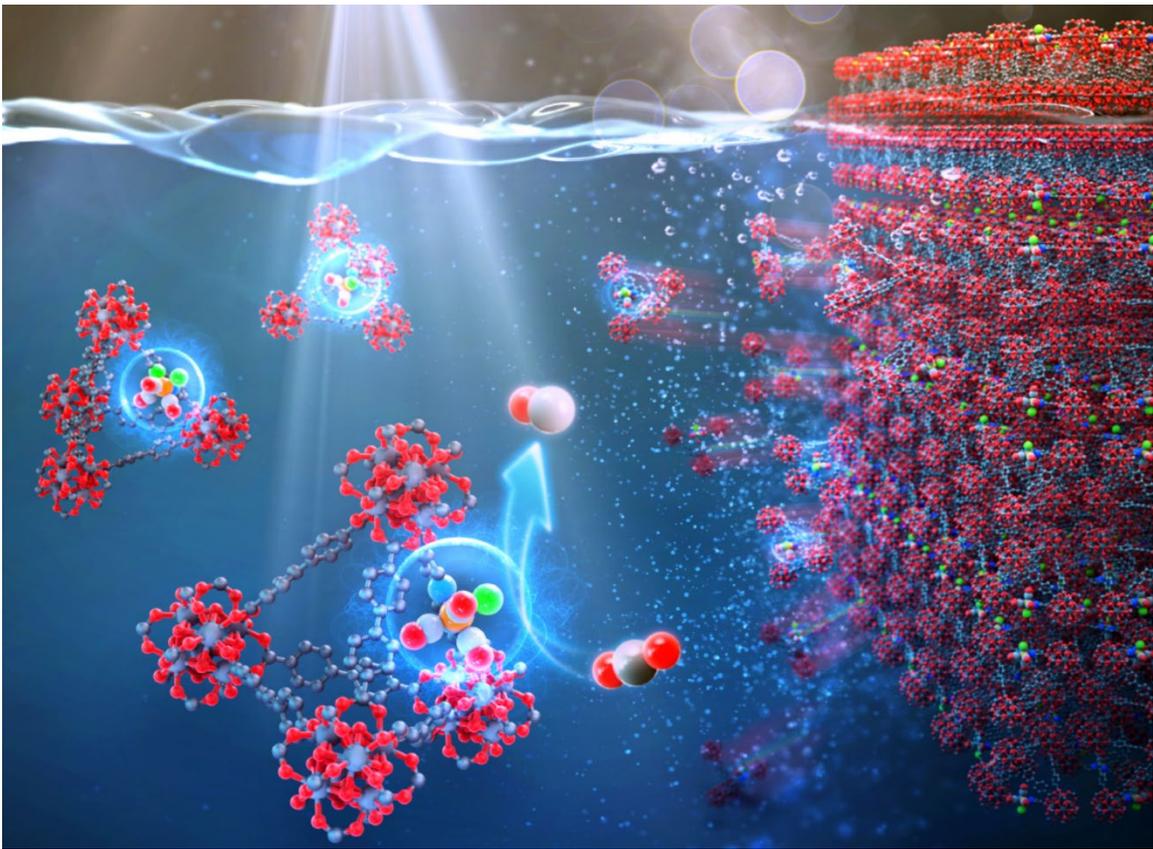
Chair: Minyoung Yoon (Kyungpook National University)

Catalytic Applications of Metal–Organic Polyhedra

Kyung min Choi

Division of Chemical and Biomolecular Engineering, Sookmyung Women's University, Korea

Development of highly active, selective, and long-lasting catalyst is sought-after demand in both heterogeneous and homogeneous catalysis. Molecular photocatalysts, having powerful features of high activity and product selectivity, have been challenged concerning their catalytic stability as they are easily transformed to inactive form and not reusable. In this report, we discovered that a discrete molecular cage of metal-organic polyhedra (MOP), structured with organic linker and inorganic joint, ultimately stabilize a molecular catalyst without losing its original catalytic activity. The molecular catalyst chemically bound to MOP preserved its high CO₂-to-CO conversion activity up to 24 hours under visible light, while its molecular form was deactivated in 2 hours. These high catalytic activity and stability are coming from the nature of MOP existing in the intermediate regime between discrete molecules and extended structures, thus combining the advantages of both homogeneous and heterogeneous catalysts.



Symposium : **PHYS1-1**

Recent Research Trends in Biophysical Chemistry

Room 404 (Live Streaming) THU 10:40

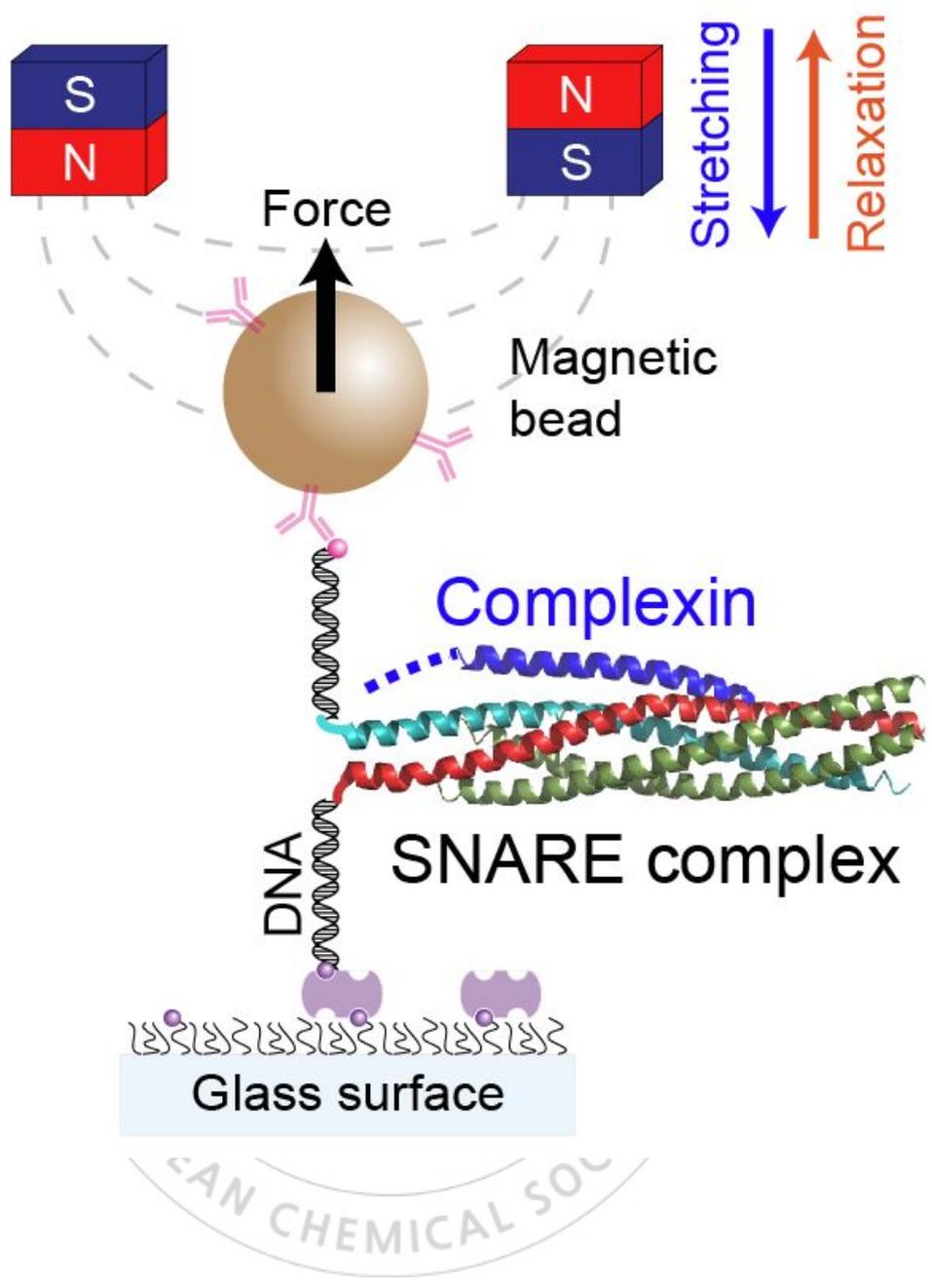
Chair: Juyong Lee (Kangwon National University)

High-speed tracking of synaptic protein interactions

Min Ju Shon

Department of Physics, POSTECH, Korea

Molecular observations of synaptic proteins provide a unique viewpoint on neurotransmission that complements electrophysiology measurements. In this talk, I will introduce molecular tweezers that can monitor the zippering of a single SNARE complex, a process that drives synaptic vesicle fusion. Using a magnetic particle, the method simultaneously manipulates and probes the fine structural dynamics of a biomolecular assembly with a nanometer-millisecond spatiotemporal resolution. Application of the method revealed partially zippered SNAREs and their interactions with other presynaptic proteins. We found that the distinct intermediate forms of a SNARE complex are differentially regulated by associated factors such as complexin and synaptotagmin. Importantly, the addition of calcium ions to the synaptotagmin-1-SNARE complex strongly drives the complete zippering of SNARE proteins, suggesting the critical role for synaptotagmin in synchronous, Ca^{2+} -triggered neurotransmission. I will also discuss how such a force application technique can be employed to address mechanical aspects of molecular neuroscience.



Symposium : **PHYS1-2**

Recent Research Trends in Biophysical Chemistry

Room 404 (Live Streaming) THU 11:00

Chair: Juyong Lee (Kangwon National University)

Prediction of Protein Structure and Interaction by Deep Learning

Chaok Seok

Division of Chemistry, Seoul National University, Korea

The history of protein structure prediction was driven by CASP competition, and recently DeepMind showed a monumental achievement in this field. One of the most interesting questions was that whether protein structures could be predicted by present biological information (protein sequences and structures) alone or not. For the last 26 years of CASP, bioinformatics approaches have been more successful in producing predictions than physics-based approaches, although some promising results were obtained by molecular dynamics simulations. In a related field of predicting protein-protein interactions represented by CAPRI and another field of predicting protein-ligand interactions, physics-based approaches have been more relevant. The absolute success of AlphaFold in CASP proved that protein structures can be predicted by exploiting present biological data at least for proteins forming stable well-defined tertiary structures. An important aspect of AlphaFold seems to be incorporation of physical insights and geometric elements into the architecture of neural network. This is because the current size of the protein structure database is not large enough compared to many other areas on which deep learning has shown great impacts. It remains to be seen how deep learning would change the field of predicting biomolecular interactions involving flexible and disordered molecules. In this talk, I will present a new deep learning approach that attempts prediction of protein structures and interactions by neural net-based free energy function, which can be potentially applied to the cases involving structural flexibilities.

Symposium : **PHYS1-3**

Recent Research Trends in Biophysical Chemistry

Room 404 (Live Streaming) THU 11:20

Chair: Sang Hak Lee (Pusan National University)

Unwinding Mechanism of Replicative Helicases: Lessons from Papillomavirus E1 Helicase

Mina Lee

Safety Measurement Institute, Korea Research Institute of Standards and Science, Korea

Ring-shaped replicative helicases are hexameric helicases that play a key role in cellular DNA replication. The replicative helicases elaborately cooperate with a multi-enzyme complex synthesizing DNA at the replication fork. Despite intensive efforts to understand this fundamental biological process, the unwinding mechanism of replicative helicases still remains unclear. Bovine papillomavirus (BPV) E1 is one of the best-known model systems for complicated eukaryotic replicative helicases. E1 is a versatile stand-alone helicase that senses and melts the viral origin (ori) and unwinds DNA. Here, we present the unwinding mechanism of E1 studied using magnetic tweezers. The results obtained with forked DNA reveal that E1 as a single hexamer (SH) is a poor helicase with low processivity and unwinding rate. The negative effect of tension on unwinding indicates that there is a strong interaction between the helicase and the non-translocating DNA strand. From high force experiments, it was found that E1 unwinds DNA while encircling both DNA strands. Next, we investigated unwinding of dsDNA with ori, where E1 has been known to be assembled as a double hexamer. Unwinding activity for the dsDNA with ori was highly dependent on the applied force; while it hardly changed at high forces, the extension rapidly decreased at low forces. Strong activity at low forces suggests that the double hexamer does not separate into two SHs during unwinding. This is, surprisingly, the opposite of what has been generally believed about replicative helicases. Robust unwinding of double hexameric E1 suggests that dimerization of SHs greatly boosts unwinding activity of E1.

Symposium : **PHYS1-4**

Recent Research Trends in Biophysical Chemistry

Room 404 (Live Streaming) THU 11:40

Chair: Sang Hak Lee (Pusan National University)

Multimodal Single-molecule and single-particle (Multimodal SMSP) imaging for nanobiological applications

Haemi Lee

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

In this talk, I will demonstrate a new multi-level wide-field imaging modality that enables the simultaneous assignment of target and non-target binding events in a detection area. The introduced multimodal single-molecule and single-particle imaging (Multimodal SMSP) system is based on parallel detection of background-free Rayleigh scattering and fluorescence (or SERS) signals that respectively generated from nano(bio)particles and their interacting small molecules. Particularly, in this presentation, the Multimodal SMSP assay will be introduced as a specific-binding identifier and quantifier to assess variable host susceptibility to a virus with the single-binding event accuracy.

Award Lecture in Division : **PHYS2-1**

Recent Trends in Spectroscopy and Dynamics

Room 404 (Live Streaming) THU 12:50

Chair: Sangwoon Yoon (Chung-Ang University)

Crystal Facet, Band Gap and Interface Junction Engineering of Photocatalysts for CO₂ Activation and Reduction with Functional Layers in Photoelectrochemical System

Young soo Kang

Department of Chemistry, Sogang University, Korea

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

have faster kinetics. The decreased amount of activation energy was determined with Tafel plots by measuring the slopes of it and semicircles of the electrochemical impedance spectroscopy (EIS) Nyquist plots at different temperatures. Nafion film coated on the surface of cathode assists the faster transport of H^+ ions to CO_2 reduction reaction sites for the simultaneous one-pot reaction of proton coupled electron transfer reactions.



Award Lecture in Division : **PHYS2-2**

Recent Trends in Spectroscopy and Dynamics

Room 404 (Live Streaming) THU 13:20

Chair: Sangwoon Yoon (Chung-Ang University)

Next generation chemical kinetics and statistical thermodynamics enabling quantitative understanding of complex nano-bio systems

Jaeyoung Sung

Department of Chemistry, Chung-Ang University, Korea

Physical or chemical processes occurring in small systems, such as living cells and nanocatalytic systems, often exhibit complex dynamics that are not easily explainable by traditional physicochemical models and theories. In this talk, we will introduce new types of kinetics and statistical thermodynamics that provide an excellent, quantitative explanation and physicochemical understanding of complex chemical dynamics observed in various biological or nanocatalytic systems. Successful applications of our approach will be demonstrated for quantitative investigations into gene expression dynamics in living cells, transport dynamics of complex fluids, reaction dynamics of nanocatalytic systems, and the nucleation and growth dynamics of nanocluster systems. These works suggest a promising new direction in physical chemical investigation into complex systems, making dynamics of complex nano-bio systems quantitatively explainable by physical chemical models and mathematical deductions.

Symposium : **PHYS2-3**

Recent Trends in Spectroscopy and Dynamics

Room 404 (Live Streaming) THU 13:50

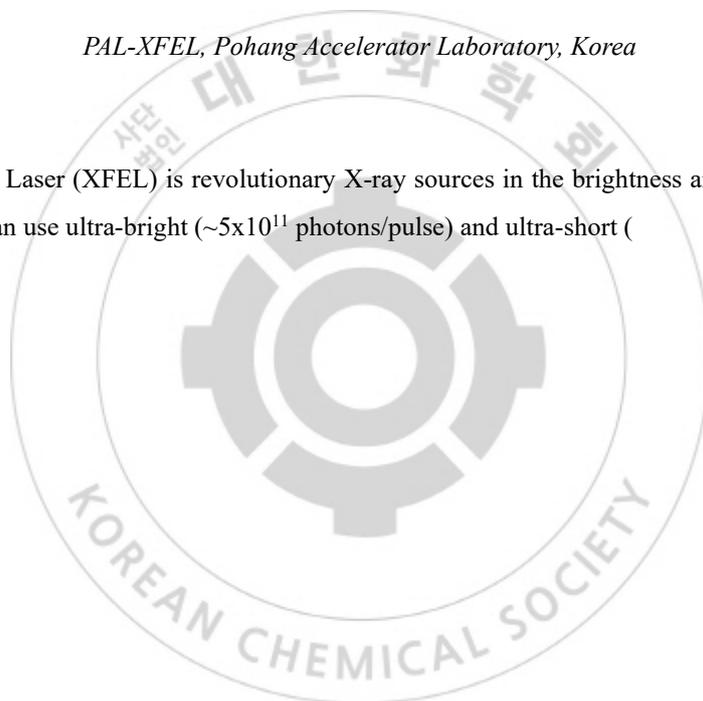
Chair: Hyungjun Kim (Incheon National University)

Time-resolved studies of chemical reaction dynamics at PAL-XFEL

Jae Hyuk Lee

PAL-XFEL, Pohang Accelerator Laboratory, Korea

X-ray free-electron Laser (XFEL) is revolutionary X-ray sources in the brightness and short pulse width. Using XFEL, we can use ultra-bright ($\sim 5 \times 10^{11}$ photons/pulse) and ultra-short (



Symposium : **PHYS2-4**

Recent Trends in Spectroscopy and Dynamics

Room 404 (Live Streaming) THU 14:10

Chair: Hyungjun Kim (Incheon National University)

Cooperation between exciton transfers and vibrations is promoted by vibrational phase synchronizations

Young Min Rhee

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

We discuss how the energy transfer and the vibrational correlations cooperate with each other based on simulations with a few numerically approximate mixed quantum classical (MQC) methods. By adopting a two-state system with locally coupled underdamped vibrations that are resonant with the electronic energy gap, we observe prominent energy dissipations from the electronic system to the vibrations, re-highlighting the role of underdamped vibrations as a temporal electronic energy buffer. This energy dissipation generates specific phase relations between the two vibrations into anti-correlations right after the initiation of the energy transfer but then into co-correlation as the transfer completes. These phase relations are interpreted as a selective activation of an anti-correlated motion of the vibrations and a subsequent deactivation by thermal energy redistribution. Furthermore, we show that a single vibration simultaneously coupled to the two electronic states with opposite phases induces a completely equivalent energy transfer dynamics as the two localized vibrations, hinting the emergence of a delocalized vibration from the localized ones. Finally, we discuss how the vibrational energy dissipation dynamics is affected by the adopted MQC approaches and warn about the increased subtlety toward properly treating dissipation effects over having reliable population dynamics.

Symposium : **PHYS2-5**

Recent Trends in Spectroscopy and Dynamics

Room 404 (Live Streaming) THU 14:30

Chair: Yoonsoo Pang (GIST)

Direct observation of structural dynamics manipulating the fate of the excited states of PDI oligomers by ultrafast time-domain Raman spectroscopy

Dongho Kim

Department of Chemistry, Yonsei University, Korea

In π -conjugated organic photovoltaic materials, an excimer state has been generally regarded as a trap state which hinders efficient excitation energy transport. But despite wide investigations of the excimer for overcoming the undesirable energy loss, the understanding of the relationship between the structure of the excimer in the stacked organic compounds and its properties remains elusive. Here, we present the landscape of structural evolution from the excimer formation to its relaxation in an archetypical perylene bisimide folda-dimer using ultrafast time-domain Raman spectroscopy. We directly probed the ultrafast structural evolution triggering the excimer formation followed by evolving into a relaxed excimer state along the intermolecular as well as solvation coordinates. This work not only showcases the ultrafast structural dynamics necessary for the excimer formation and control of excimer characteristics but also provides important criteria for designing the π -conjugated organic molecules.

Symposium : **PHYS2-6**

Recent Trends in Spectroscopy and Dynamics

Room 404 (Live Streaming) THU 14:50

Chair: Yoonsoo Pang (GIST)

Excited state molecular dynamics based on machine learning approach

Seung Kyu Min

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

Excited state molecular dynamics (ESMD) is an effective computational tool to understand photochemical/physical phenomena such as photosynthesis, vision process, photovoltaics and light-driven chemical reactions. The conventional ESMD simulation within mixed quantum-classical frameworks propagates classical nuclear trajectories on multiple electronic states, so-called Born-Oppenheimer electronic states, with nonadiabatic coupling among them. Since the trajectories depends on the quality of excited states, fairly accurate electronic excited state calculations should be performed to reach reasonable accuracies. Therefore, a long time simulation of ESMD is practically impossible due to computational costs. Nowadays, computational chemists try to replace high quality quantum chemical calculation as machine learning approaches. Lots of research works have been published so far to combine machine learning approaches and quantum chemical calculations. In this presentation, we present our recent work on excited state molecular dynamics simulation based on machine learning approach to overcome singularity problems in the presence of conical intersections. We propose learning diabatic Hamiltonian from ensemble density functional theory instead of adiabatic Hamiltonian.

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

Recent Trends in Theoretical and Computational Chemistry

Room 404 (Live Streaming) THU 15:20

Chair: Sangwoon Yoon (Chung-Ang University)

Computer Simulation Studies of Biological and Material Systems

Rakwoo Chang

Department of Applied Chemistry, University of Seoul, Korea

In this talk, we will discuss several computer simulation studies of biological and material systems using various molecular models and methods. The first topic is the interaction between testis-expressed gene 14 (TEX14) and the midbody protein centrosomal protein (CEP55) in cell division using the well-tempered metadynamics simulation techniques. The binding Gibbs free energy surface obtained by the metadynamics simulation is in good agreement with the corresponding experimental results. In the second topic, the morphological stability of organic photovoltaic (OPV) cells is explored using both atomistic and coarse-grained molecular dynamics simulation studies. It is observed that the number of components in the OPV system plays a significant role in the morphological stability of OPV by delaying the spontaneous phase separation.

Symposium : **PHYS3-2**

Recent Trends in Theoretical and Computational Chemistry

Room 404 (Live Streaming) THU 15:50

Chair: Kyoung Chul Ko (Chonnam National University)

Exploring Chemical Space using Machine Learning

Yousung Jung

Korea Advanced Institute of Science and Technology, Korea

Discovery of new molecules and material with desired properties is the ultimate goal of materials research. To date, a generally successful strategy has been to use chemical intuition and empirical rules to design new materials, but these conventional approaches require a significant amount of time and cost due to almost unlimited combinatorial possibilities of inorganic materials in chemical space. A promising way to significantly accelerate the latter process is to incorporate all available knowledge and data to plan the synthesis of the next material. In this talk, I will present several directions to use informatics to efficiently explore chemical space. I will first describe methods of machine learning for fast and reliable predictions of materials and molecular properties that can replace density functional calculations, an essential component needed for large scale materials design. With these tools in place for property evaluation, I will next present a few initial frameworks that we have recently developed to allow generative inverse design of inorganic crystals with optimal target properties, either in the compositional space or structural space. I will finally discuss several challenges and opportunities that lie ahead for further developments of accelerated materials acceleration platform, including retrosynthesis and synthesizability of molecules and materials.

Symposium : **PHYS3-3**

Recent Trends in Theoretical and Computational Chemistry

Room 404 (Live Streaming) THU 16:10

Chair: Kyoung Chul Ko (Chonnam National University)

Geometry Optimizations with Large Active Spaces in Highly Correlated Systems

Jae Woo Park

Department of Chemistry, Chungbuk National University, Korea

Accurate descriptions of electron correlation lie at the heart of modern quantum chemistry methods. In particular, there are cases that one should include multiple electronic configurations in calculations to obtain satisfactory accuracy. The complete active-space (CAS) is probably the dominant way of determining the list of electronic configurations (Slater determinants). However, if the number of active orbitals is large (usually >16), it is impossible to compute with the CAS approach due to the exponential growth of the determinant numbers. The selected CI (SCI) method stochastically determines the list for such calculations. Here, I present recent progress on developing formalism and computer codes for molecular geometry optimizations with large active space using the adaptive sampling configuration interaction (ASCI) method by Head-Gordon, Whaley, and coworkers. I mainly introduce the analytical gradient theories for adaptive sampling configuration interaction self-consistent field (ASCI-SCF) and its second-order perturbatively corrections (ASCI-SCF-PT2).

Symposium : **PHYS3-4**

Recent Trends in Theoretical and Computational Chemistry

Room 404 (Live Streaming) THU 16:30

Chair: Chang Yun Son (POSTECH)

Theta-chain in confined space and its implication to biopolymers

Changbong Hyeon

School of Computational Sciences, Korea Institute for Advanced Study, Korea

When compressed in a slit of width D , a theta-chain whose size (R_0) scales as $R_0 \sim aN^{1/2}$, expands in the lateral direction as $R_{\parallel} \sim aN^{\nu(a/D)^{2\nu-1}}$. Provided that the theta condition is strictly maintained throughout the compression, the well-known scaling exponent of Θ -chain in two dimensions, $\nu = 4/7$, is anticipated upon a perfect confinement. However, numerics shows that upon increasing compression, the exponent ν gradually deviates from $\nu = 1/2$ and plateaus at $\nu = 3/4$, the exponent associated with the self-avoiding walk in two dimensions. Using both theoretical considerations and numerics, we argue that it is highly nontrivial to maintain the Θ condition under confinement because of two major effects. First, as the dimension is reduced from three to two dimensions, the contributions of higher order virial terms, which can be ignored in three dimensions at large N , become significant, making the perturbative expansion used in Flory-type approach inherently problematic. Second and more importantly, the geometrical confinement, which is regarded as an applied external field, alters the second virial coefficient (B_2) changes from $B_2 = 0$ (Θ condition) in free space to $B_2 > 0$ (good-solvent condition) in confinement. Our study offers better understanding of the confinement effect on the conformation of a single biopolymer chain.

Symposium : **PHYS3-5**

Recent Trends in Theoretical and Computational Chemistry

Room 404 (Live Streaming) THU 16:50

Chair: Chang Yun Son (POSTECH)

Effect of curvature on diffusion-controlled reactions and its application to the Berg-Purcell ligand-binding model

Changsun Eun

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Although many surface reactions occur on curved surfaces, the effect of curvature on surface reactions has not been discussed until recently. In this study, we analyze a simple model in which a diffusion-controlled bimolecular reaction occurs on a curved surface. Upon solving the diffusion equation numerically, we find that the rate constant is a nonlinear function of the surface curvature and exhibits a maximum at a certain curvature. Based on this finding, we theorize that a quadratic equation can reproduce these features and demonstrate that this theory is in agreement with the result from our numerical calculation. Moreover, we discuss the application of our theory to improve the rate constant formula in the Berg-Purcell ligand-binding model of a spherical cell membrane covered by multiple receptors. Overall, our study reveals the role of curvature in surface reactions and the influence of the size, number, and spatial arrangement of reactive patches on a sphere on reaction kinetics.

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

Convergence Analytical Chemistry for Disease Diagnosis

Room 301 (Live Streaming) THU 14:30

Chair: Tae-Young Kim (GIST)

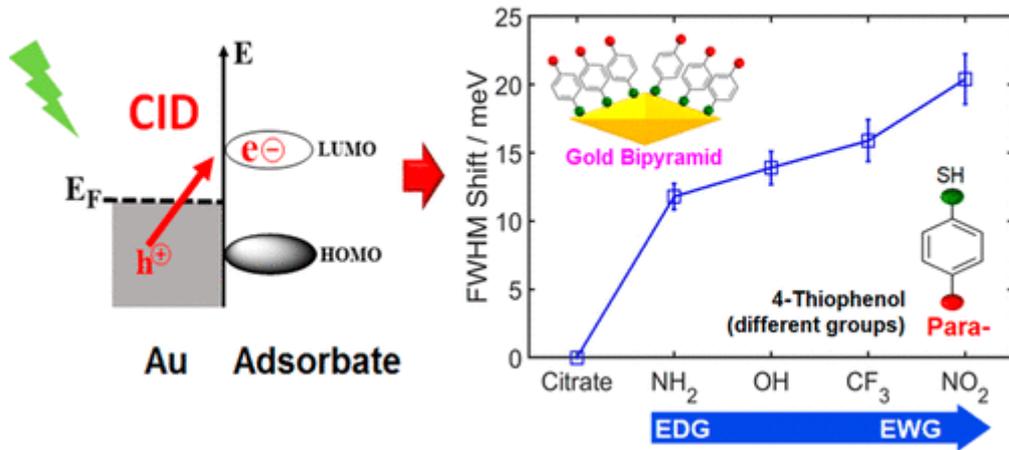
Tuning Chemical Interface Damping in Single Gold Nanorods

Ji won Ha

Department of Chemistry, University of Ulsan, Korea

Recently, chemical interface damping (CID) has been proposed as a new plasmon damping pathway based on interfacial hot-electron transfer from metal to adsorbate molecules.[1] It has been considered essential, owing to its potential implications in efficient photochemical processes and sensing experiments. However, thus far, studies focusing on controlling CID in single gold nanoparticles have been very limited, and in situ reversible tuning has remained a considerable challenge. In this scanning electron microscopy-correlated dark-field (DF) scattering study, the CID was controlled by focusing on the electronic nature of disubstituted benzene rings acting as adsorbates, as well as the effects of sharp tips on gold bipyramids (AuBPs) with similar aspect ratios to those of gold nanorods (AuNRs). Electron withdrawing groups (EWGs) on the adsorbates induce larger homogeneous LSPR linewidths compared to those of electron donating groups (EDGs).[2] Furthermore, in our scanning electron microscopy-correlated DF spectroscopic measurements and density functional theory calculations, cucurbit[7]uril (CB[7])-based host-guest supramolecular interactions were employed for the first time to examine and control the CID process using monoamine-functionalized CB[7] (CB[7]-NH₂) attached to single AuNRs.[3] A new method of in situ tuning of CID through the CB[7]-oxaliplatin complexation, which can result in the variation of chemical nature and electronic properties of adsorbates, was presented. In addition, in situ tuning of CID was demonstrated through the competitive release of the oxaliplatin guest from the oxaliplatin@CB[7] complex, which was then replaced by a competitor guest of spermine at sufficient amount. Furthermore, nuclear magnetic resonance experiments confirmed that the release of the guest is the consequence of adding salt (NaCl). Thus, in situ reversible tuning of CID in single AuNRs was achieved through successive steps of encapsulation and release of a guest on the same AuNR in a flow cell.

Interfacial Electronic Effect on Chemical Interface Damping



Symposium : **ANALI-1**

Convergence Analytical Chemistry for Disease Diagnosis

Room 301 (Live Streaming) THU 13:00

Chair: Young-Kwan Kim (Dongkuk University)

Advanced strategies for miRNA detection based on Graphene oxide

Jieon Lee

Predictive toxicology department, Korea institute of toxicology, Korea

MicroRNAs (miRNAs), short non-coding RNAs, have emerged as promising next-generation biomarkers of diverse diseases. In general, conventional quantitative real-time PCR and miRNA microarray methods have been utilized for the quantitative detection of miRNA. However, owing to their complicated procedures and expensive reagents/instruments, these methods cannot be widely applied by medical experts such as doctors and nurses, and are thus limited for practical clinical application. In this presentation, we introduce graphene oxide (GO)-based optical sensing strategies for miRNA with enhanced sensitivity, specificity, user-friendliness, scalability, and portability. They are fundamentally based on the physical/chemical/optical properties of GO and newly-designed functional DNA probes for miRNAs. They have potential for use in point-of-care testing (POCT), multiplex imaging, and reliable screening. We believe that these new GO-based sensors can be a suitable tool for miRNA-based practical diagnostics of diseases, and provides a valuable resource for basic and applied research.

Symposium : **ANAL1-2**

Convergence Analytical Chemistry for Disease Diagnosis

Room 301 (Live Streaming) THU 13:20

Chair: Young-Kwan Kim (Dongkuk University)

Development of Nucleic Acid Nanoengineering-based Biosensor for Virus Detection

Taek Lee

Department of Chemical Engineering, Kwangwoon University, Korea

Since 2010, nucleic acid nanoengineering has been attracted for cancer treatment, gene delivery, bioimaging and therapeutic applications. Recently, the field of nucleic acid nanoengineering has been extended to biosensor and in vitro diagnostics because of high specificity to target bioprobe, thermodynamic stability of structure and easy-to-tailoring for embodying the functionality. Among them, virus is one of the harmful pathogens to human due to fast infection, mutants and high fatal rate. To detect the virus effectively, the author fabricated multi-functional nucleic acid-nanoparticle hybrid for virus biosensor application. As a multi-functional bioprobe, the DNA 3WJ was introduced. Each fragment of DNA 3WJ was rolled to recognition part (viral protein detection aptamer), signal transduction part and immobilization part, respectively. Each fragment was assembled to form the DNA 3WJ for virus detection and the assembled structure was confirmed by various techniques including the electrophoresis, atomic force microscopy and others. The nucleic acid nanoengineering will pave the way for various virus detection platforms./Acknowledgements: This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2018R1D1A1B07049407) by Korea Environment Industry&Technology Institute(KEITI) through the program for the management of aquatic ecosystem health, funded by Korea Ministry of Environment(MOE).(2020003030001) by the Industrial Core Technology Development Program(20009121, Development of early diagnostic system of peritoneal fibrosis by multiplex detection of exosomal nucleic acids and protein markers) funded by the Ministry of Trade, Industry and Energy (MOTIE, Korea)

Symposium : **ANALI-3**

Convergence Analytical Chemistry for Disease Diagnosis

Room 301 (Live Streaming) THU 13:40

Chair: Young-Kwan Kim (Dongkuk University)

An NIR dual-emitting/absorbing inorganic compact pair: a self-calibrating LRET system for homogeneous virus detection

Joonseok Lee

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

Many conventional optical biosensing systems use a single responsive signal in the visible light region, limiting their practical applications as the signal can be readily perturbed by various external environmental factors. Herein, a near-infrared (NIR)-based self-calibrating luminescence resonance energy transfer (LRET) system was developed for background free detection of analytes in homogeneous sandwich-immunoassays. The inorganic LRET pair comprised NIR dual-emitting lanthanide-doped nanoparticles (LnNPs) as a donor and NIR absorbing LnNPs as an acceptor, which had a narrow absorption peak (800 nm) and showed long-term stability, enabling stable LRET with built-in self-calibrating signal. Screened single-chain variable fragments (scFvs) were used as target avian influenza virus (AIV)-binding antibodies to increase LRET efficiency in sandwich-immunoassays. The compact sensor platform successfully detected AIV nucleoproteins with a 0.38 pM limit of detection in HEPES buffer and 56 clinical samples. Hence, inorganic LnNP pairs may prove effective in self-calibrating LRET systems in the background-free NIR region.

Symposium : **ANAL1-4**

Convergence Analytical Chemistry for Disease Diagnosis

Room 301 (Live Streaming) THU 14:00

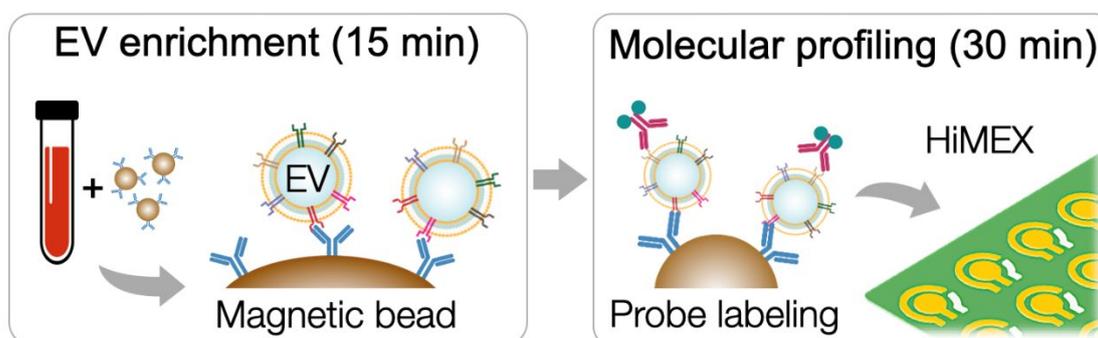
Chair: Young-Kwan Kim (Dongkuk University)

Immunomagnetic Electrochemical Sensor for Extracellular Vesicle Analysis and Disease Diagnosis

Jongmin Park

department of Chemistry, Kangwon National University, Korea

Extracellular vesicles, including exosomes, are nanoscale membrane particles that carry molecular information on parental cells. They are being pursued as biomarkers of various diseases, especially cancer that are difficult to detect or serially follow. To solve this issue, we developed a compact sensor technology for rapid, on-site exosome screening. The sensor is based on an integrated magneto–electrochemical assay: exosomes are immunomagnetically captured from patient samples and profiled through electrochemical reaction. By combining magnetic enrichment and enzymatic amplification, the approach enables (i) highly sensitive, cell-specific exosome detection and (ii) sensor miniaturization and scale-up for high-throughput measurements. We demonstrated this system to screen extracellular vesicles in human body fluids such as plasma or urine samples from patients with ovarian cancer¹, kidney transplant rejection² and colorectal cancer patients³. The sensor allowed for the simultaneous profiling of multiple protein markers within an hour, outperforming conventional methods in assay sensitivity and speed.



Symposium : **ANAL2-1**

Super-resolution Imaging Technology beyond the Limit of Optical Microscopy and Various Applications

Room 301 (Live Streaming) THU 15:10

Chair: Seungah Lee (Kyung Hee University)

Overcoming Photobleaching in Single-molecule Localization Microscopy by Exchangeable Probes

Sang-Hee Shim

Department of Chemistry, Korea University, Korea

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

Symposium : **ANAL2-2**

Super-resolution Imaging Technology beyond the Limit of Optical Microscopy and Various Applications

Room 301 (Live Streaming) THU 15:30

Chair: Seungah Lee (Kyung Hee University)

Super-resolution imaging by photoactivated atomic force microscopy

Yunseok Kim

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

Imaging intrinsic optical absorption properties of materials with optical microscopy (OM) is strongly limited by the optical diffraction limit. On the other hand, while nanoscale fluorescence OM has become crucial for investigating the morphologies of materials, it is not suitable for imaging optical absorption and further requires the use of additional fluorescent molecules for exploring biological materials. In this presentation, we demonstrate super-resolution visible photoactivated atomic force microscopy (pAFM) based on the thermoelastic effects induced by pulsed laser irradiation. Since it can sense intrinsic optical absorption with ~ 8 nm resolution, the resolution can be further improved down to ~ 8 nm. Moreover, pAFM can detect not only the first harmonic response but also the second harmonic response based on the nonlinear effect. The pAFM allows exploring single gold nanospheres, nanowires, and biological materials at the nanoscale resolution. We believe that the pAFM would be broadly useful and could have wide impacts in such fields as chemistry, materials science, physics, biology and electronics.

Symposium : **ANAL2-3**

Super-resolution Imaging Technology beyond the Limit of Optical Microscopy and Various Applications

Room 301 (Live Streaming) THU 15:50

Chair: Seungah Lee (Kyung Hee University)

Oblique STORM for thick biological samples

Jeongmin Kim

Department of Applied Bioengineering, Seoul National University, Korea

Optical microscopy, by visualizing small worlds beyond human vision, has revolutionized many branches of science including biology. These days optical microscopes also play a key role as a major metrology tool in engineering fields and micro/nano manufacturing industry. Yet, the development of optical microscopy itself is still an active area of research as the end user's demand for new or improved imaging capabilities continues to increase. One of the research directions is super-resolution, achieving imaging resolution below 100 nm, which is at least two-fold better than the diffraction limited resolution in conventional optical microscopy. Single molecule localization microscopy, a.k.a. STORM or PALM, has provided superior spatial resolution down to 20 nm since 2006, but the optical configuration of typical STORM/PALM setups has limited its application mostly to thin biological samples like adherent cells. Here, I will present an oblique STORM platform developed for thicker biological samples such as tissues or small intact animals. Our STORM method enables deep tissue investigation in a multicolor and volumetric super-resolution manner, broadly expanding applicability of STORM/PALM techniques beyond the cellular level.

Symposium : **ANAL2-4**

Super-resolution Imaging Technology beyond the Limit of Optical Microscopy and Various Applications

Room 301 (Live Streaming) THU 16:20

Chair: Seungah Lee (Kyung Hee University)

Shaping light for bio-imaging

Jung-Hoon Park

Biomedical Engineering, Ulsan National Institute of Science and Technology, Korea

Advances in bio-imaging have enable observation of light at higher spatiotemporal resolutions. In general, the spatiotemporal resolution is fixed across the field of view. This comes as a limitation for instance, when we want to apply fluorescence based superresolution techniques. Since all fluorescence based superresolution technologies developed to date induce a loss in temporal resolution, the temporal resolution is decreased across the entire field of view. Here, we demonstrate how we can shape the illumination beam to enable different imaging characteristics across the field of view simultaneously. For example, by illuminating selective sinusoidal illumination patterns, we realize tunable SIM, a novel dynamic adaptive structured illumination microscope which realizes varying spatiotemporal resolutions across the field of view that can adapt to the user's needs. We further discuss how we can use custom illumination to enable stroboscopic or high dynamic range imaging for advanced bio imaging applications.

Symposium : **ANAL2-5**

Super-resolution Imaging Technology beyond the Limit of Optical Microscopy and Various Applications

Room 301 (Live Streaming) THU 16:40

Chair: Seungah Lee (Kyung Hee University)

Single-molecule sensing and imaging by spectrally resolved super-resolution microscopy

Doory Kim

Department of Chemistry, Hanyang University, Korea

Recent advances in single-molecule spectroscopic imaging techniques, such as spectrally resolved stochastic optical reconstruction microscopy (SR-STORM), have been effective for obtaining detailed spectral information at the molecular level. However, its application for single-molecule sensing is highly challenging owing to its complicated configuration and limited spectral information. In this study, we demonstrated single-molecule polarity sensing by combining SR-STORM with the solvatochromic dye. The spatial and spectral resolutions of the custom-built grating-based SR-STORM were examined for various color ranges of fluorescent dyes, and this approach was successfully applied for sensing nanoscale local polarity of various organic solvent molecules and surfactant molecules. Furthermore, we demonstrated that the proposed method effectively distinguished the different polarities of functional groups within surfactant molecules at the single-molecule level. We anticipate that the proposed approach can be combined with other chromic molecules for application to many other chemical systems.

Symposium : **LIFE1-1**

Biochemical Approaches on Alzheimer's Disease Research

Room 305 (Live Streaming) THU 13:00

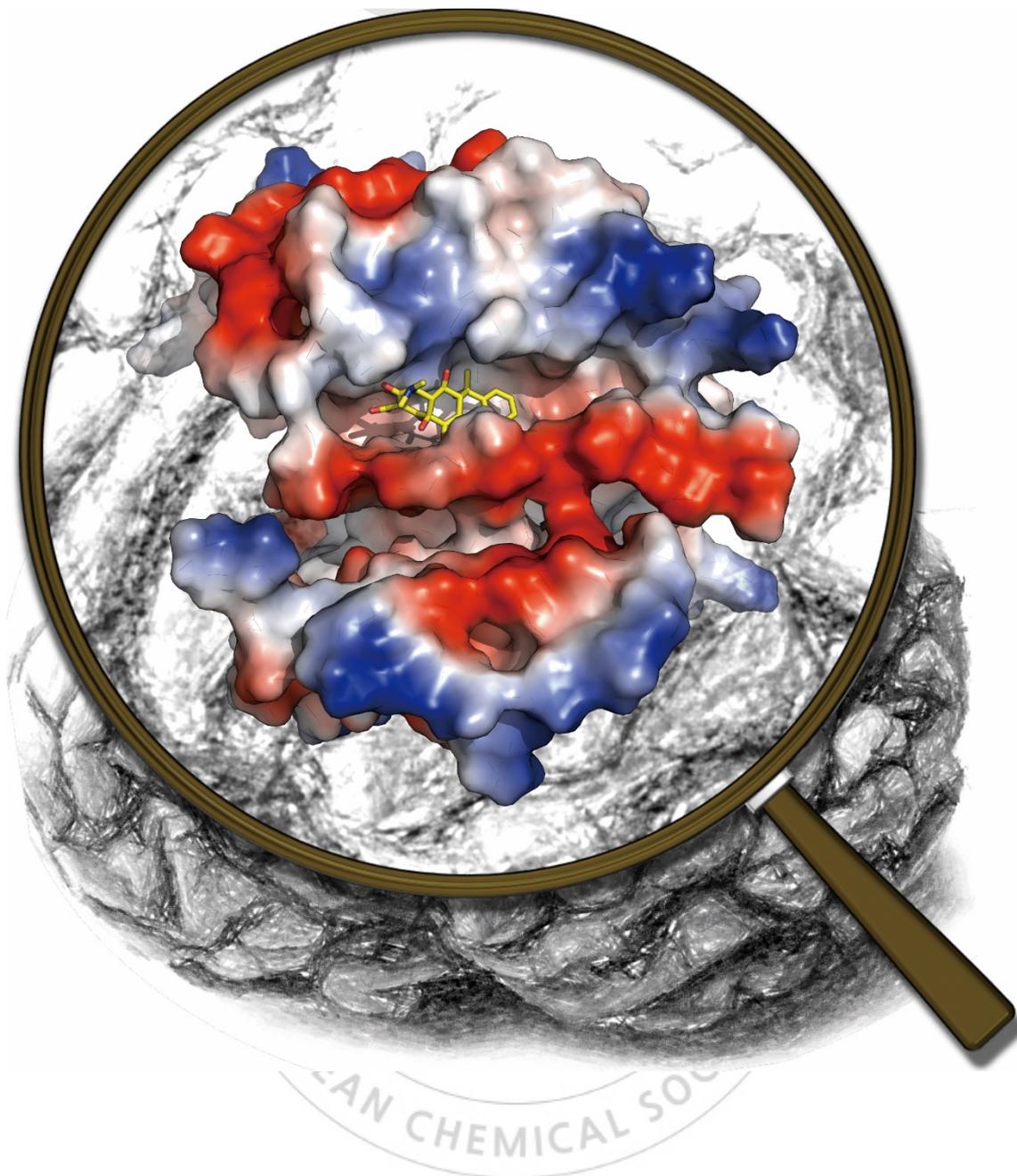
Chair: Jun-Seok Lee (Korea University)

Chemical-Driven Disaggregation of Misfolded Proteins For Alzheimer Disease

YoungSoo Kim

Department of Pharmacy, Yonsei University, Korea

According to the amyloid hypothesis, Alzheimer's disease (AD) is caused by abnormal production, consequent toxic aggregation, and insufficient removal of amyloid- β ($A\beta$) in the brain. Although measurements of amyloid burden in the central nervous system became a standard diagnostic method of the disease, drug candidates targeting the $A\beta$ cascade have never been approved for clinical uses yet. As a result, many have suspected the validity of $A\beta$ as a therapeutic target due to disappointments of chemical drug candidates. However, promising clinical trials of immunotherapy candidates of $A\beta$ clearance mechanism support the view that the amyloid cascade is the pathological culprit of AD. Our primary aim in this review is to discuss a chance to develop chemical drugs to clear $A\beta$ oligomers and plaques from the brain, just like the immunotherapy, as when structural understanding of misfolded $A\beta$ is still unknown. Here, we introduced a drug discovery methodology to develop chemical mimics of those antibody drug candidates and our drug candidates.



Symposium : **LIFE1-2**

Biochemical Approaches on Alzheimer's Disease Research

Room 305 (Live Streaming) THU 13:20

Chair: Jun-Seok Lee (Korea University)

Visualization of Tau Oligomerization in the Brain

Yun Kyung Kim

Chemical biology, Alzheimer's Disease, Korea

Accumulation of abnormal tau aggregates in the brain is a pathological hallmark of multiple neurodegenerative disorders including Alzheimer's disease. Increasing evidence suggests that soluble tau aggregates play a key role in tau pathology as neurotoxic species causing neuronal cell death and act as prion-like seeds mediating tau propagation. Despite the pathological relevance, there is a paucity of methods to monitor tau oligomerization in the brain. As a tool to monitor tau self-assembly in the brain, we generated a novel tau transgenic mouse, named TauP301L-BiFC. By introducing bimolecular fluorescence complementation technique to human tau containing a P301L mutation, we were able to monitor and quantify tau self-assembly, represented by BiFC fluorescence in the brains of transgenic TauP301L-BiFC mice. TauP301L-BiFC mice showed soluble tau oligomerization from 3 months, showing significantly enriched BiFC fluorescence in the brain. Then, massive tau fragmentation occurred at 6 months showing dramatically decreased TauP301L-BiFC fluorescence. The fragmented tau species served as a seed for insoluble tau aggregation. In a result, insoluble TauP301L-BiFC aggregates coaggregated with endogenous mouse tau accumulated in the brain, showing subsequently increased BiFC fluorescence from 9 months. Neuronal degeneration and cognitive deficits were observed from 12 months of age. TauP301L-BiFC mouse model demonstrated that methylene blue reduced the amount of soluble tau oligomers in the brain, resulting in the prevention of cognitive impairments. We assure that TauP301L-BiFC mice are a bona-fide animal tool to monitor pathological tau oligomerization in AD and other tauopathies.

Symposium : **LIFE1-3**

Biochemical Approaches on Alzheimer's Disease Research

Room 305 (Live Streaming) THU 13:40

Chair: Jun-Seok Lee (Korea University)

Biochemical Findings of the Double-Hit Model for Tau Aggregation

Min Jae Lee

College of Medicine, Biochemistry, Seoul National University, Korea

The tau protein is a highly soluble and natively unfolded protein. Under pathological conditions, tau undergoes multiple post-translational modifications (PTMs) and conformational changes to form insoluble filaments, which are the proteinaceous signatures of tauopathies. To dissect the crosstalk among tau PTMs during the aggregation process, we phosphorylated and ubiquitylated recombinant tau in vitro using GSK3beta and CHIP, respectively. The resulting phospho-ub-tau contained conventional polyubiquitin chains with lysine 48 linkages, sufficient for proteasomal degradation, whereas unphosphorylated ub-tau species retained only one–three ubiquitin moieties. Mass-spectrometric analysis of in vitro reconstituted phospho-ub-tau revealed seven additional ubiquitylation sites, some of which are known to stabilize tau protofilament stacking in the human brain with tauopathy. When the ubiquitylation reaction was prolonged, phospho-ub-tau transformed into insoluble hyperubiquitylated tau species featuring fibrillar morphology and in vitro seeding activity. Our biochemical findings point to a “multiple-hit model,” where sequential events of tau phosphorylation and hyperubiquitylation function as a key driver of the fibrillization process, thus indicating that targeting tau ubiquitylation may be an effective strategy to alleviate the course of tauopathies.

Symposium : **LIFE1-4**

Biochemical Approaches on Alzheimer's Disease Research

Room 305 (Live Streaming) THU 14:00

Chair: Jun-Seok Lee (Korea University)

A therapeutic strategy for synaptic and organelle dysfunction in Alzheimer's Disease

Seongsoo Lee

Gwangju Center, Korea Basic Science Institute, Korea

Amyloid plaques and neurofibrillary tangles were recognized more than a century ago as the pathological hallmarks of Alzheimer's disease (AD). However, the relative contribution of these two lesions to disease pathogenesis and their mechanistic relationship are still topics of intense debate in the field. This is partly due to our incomplete understanding of earliest molecular changes, when there is opportunity for reversal. Our goals are to use the *Drosophila* models to dissect out the signalling pathways that connect APP (amyloid precursor protein) aberration with tau abnormality and synaptic dysfunction and to identify potential therapeutic target. Using loss-of-function and gain-of-function genetic analyses and biochemical approaches, we demonstrated that PAR-1 (partitioning defective 1) acts as a physiological tau kinase and that PAR-1 action is critical in conferring tau neurotoxicity. We also suggested that phosphor-dependent ubiquitination and degradation of PAR-1 regulates synaptic morphology and tau-mediated amyloid beta toxicity in *Drosophila*. This provided mechanistic insights into the molecular events involved in tau regulation and identified PAR-1 kinase as a new player in AD and a potential target. Interestingly, PAR-1 is activated in other disease the presence of tau-independent pathogenic mechanisms initiated by PAR-1. This raises the potential of PAR-1 kinase as a drug target for AD as well as other neurodegenerative diseases that present with synaptic and organelle dysfunction. Successful completion of our goals will be facilitated by innovative methods and strategies for live visualizing and manipulating organelle distribution in vivo in *Drosophila* and in human neuronal models of AD.

Symposium : LIFE1-5

Biochemical Approaches on Alzheimer's Disease Research

Room 305 (Live Streaming) THU 14:20

Chair: Jun-Seok Lee (Korea University)

Chemical Tools and 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 ($A\beta$) 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 $A\beta$ plaque and likely contribute to $A\beta$ neurotoxicity and oxidative stress. ROS have been shown to increase the rate of $A\beta$ 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.⁴⁻¹¹References 1. *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 : **LIFE2-1**

Recent Trends in Omics Research

Room 305 (Live Streaming) THU 15:00

Chair: Jong-Seo Kim (Seoul National University)

A single cell atlas of human thymus across development and aging defines dynamics of T cell development

Jongeun Park

Graduate School of Medical Science and Engineering, Korea Advanced Institute of Science and Technology, Korea

The thymus is the critical organ for T-cell development and T-cell receptor (TCR) repertoire formation, which shapes the landscape of adaptive immunity. While the thymus has been extensively studied using diverse animal models, the detailed atlas of human thymus is required to understand human immunity. To provide a comprehensive atlas of thymic cells across human life, we performed scRNAseq using dissociated cells from human thymus during development, childhood and adult life. We identified more than 50 different cell states in the human thymus, which dynamically change in abundance and gene expression profiles across development, paediatric and adult life. We computationally predicted the trajectory of human T-cell development from early progenitors in the hematopoietic fetal liver into diverse mature T cell types. Using this trajectory, we constructed a framework of putative transcription factors driving T-cell fate determination. Our single-cell transcriptome profile of the thymus across human lifetime and across species provides a high-resolution census of T-cell development within the native tissue microenvironment. Systematic comparison between human and mouse thymus highlights human-specific cell states and gene expression signatures. Our detailed cellular network of the thymic niche for T-cell development will aid the establishment of in vitro organoid culture models that faithfully recapitulate human in vivo thymic tissue.

Symposium : **LIFE2-2**

Recent Trends in Omics Research

Room 305 (Live Streaming) THU 15:30

Chair: Jong-Seo Kim (Seoul National University)

Acetate metabolism characterizes malignancy, metabolic nature, and prognosis of liver cancer

Sunghyok Park

College of Pharmacy, Seoul National University, Korea

Acetate is an important nutrient that can be used as a carbon source in cell metabolism. In order for acetate to be used in cells, expression of ACSS2 is required for being activated as acetyl-CoA, and the use of acetate varies depending on the amount of ACSS2 expression. However, it is still unclear to what extent acetate can be used in cells with increased expression of ACSS2 and how it can affect the malignancy of cancer. We confirmed that exogenous acetate can be actively used in most metabolic pathways in normal physiological state in cells with increased expression of ACSS2. Exogenous acetate was concentrated in anabolism such as fatty acid de novo synthesis, and lipid accumulation was confirmed at both the metabolite and gene level. It was confirmed that proliferation and lipid synthesis were reduced by using ACSS2 siRNA and inhibitor, and that it was specifically glycolytic when ACSS2 siRNA was treated. The orthotopic mouse model confirmed the similarity with cell level metabolism and confirmed that cancer growth is active and metastatic at ACSS2 low. The bioinformatics data of Liver cancer patients confirmed that ACSS2 low was associated with cancer malignancy and reduced survival. Among them, when genetic analysis was performed by classifying them based on 13% of patients who were difficult to treat, stable lipid anabolism was found in patients with less-malignant ACSS2 high. Increased use of acetate in less-malignant patients was also confirmed by PET-CT imaging in liver cancer patients. Our study suggests the possibility of stratifying liver cancer patients and finding appropriate treatment targets by correlating the metabolism of acetate to anabolism and less-malignancy.

Symposium : LIFE2-3

Recent Trends in Omics Research

Room 305 (Live Streaming) THU 16:00

Chair: Jong-Seo Kim (Seoul National University)

Host dietary amino acids determine gut symbiont alpha-galactosylceramide structures rendering unique immunomodulatory functions

Sungwhan Oh^{*}, Jamie Rossjohn^{1,*}, Seung Bum Park^{2,*}, Dennis Kasper^{3,*}

CETRI, Brigham and women's Hospital/Harvard Medical School, United States

¹*Biochemistry and Molecular Biology, Monash University, Australia*

²*Division of Chemistry, Seoul National University, Korea*

³*Immunology, Harvard Medical School, United States*

Symbiotic microbiota-derived small molecules play an important role in intestinal immune development and regulation, however, the understanding of structure-activity relationship is limited. Taking advantage of targeted metabolomic analysis with authentic standards, we unambiguously assigned the structures of immunomodulatory alpha-galactosylceramides from the human symbiont *Bacteroides fragilis* (BfaGCs). Characteristic branching of BfaGCs is the result of incorporation of branched-chain amino acids (BCAA) and symbiotic *B. fragilis* can uptake BCAAs from the host diet in the gut. Mice monocolonized with a *B. fragilis* knockout strain that cannot metabolize BCAA showed reduction in branched-chain BfaGC and impaired colonic NKT cell regulation, implying structure-specific immunomodulatory activity. NKT activation assay with synthetic BfaGC variants confirmed that the sphinganine chain branching is a critical determinant of activity. BfaGCs not only have unique immunomodulatory gene expression signatures and effector functions of stimulated NKT cells and APCs, which is distinct from the responses to the canonical Th1 or Th2-skewed NKT agonists, but also showed sphinganine branching-specific responses in APCs and NKT cells among them. Co-crystal structure and affinity analyses of the CD1d-BfaGC-NKT cell receptor complexes confirmed the unique interaction of BfaGCs as CD1d-restricted ligands. Untangling host-microbiota-diet complexity, we present structural- and molecular-level explanation of unique immunomodulatory action of endobiotic (symbiont-originated) metabolites.

Symposium : **LIFE2-4**

Recent Trends in Omics Research

Room 305 (Live Streaming) THU 16:30

Chair: Jong-Seo Kim (Seoul National University)

High-resolution mapping of RNA-binding sites/regions via chemical tools

Jong-Seo Kim

School of Biological Sciences, Seoul National University, Korea

Mass spectrometry (MS) based proteomics has been used to elucidate the RNA-interactome in various biological systems. However, the profiling resolution of RNA-binding sites or domains still remains in poor and vague stage. Here, I will present a couple of recently developed methods for high-resolution mapping of RNA-binding sites or regions using chemical tools; 1) RBS-ID and 2) FAX-RIC. RNA-binding site (RBS)-ID is a method that uses hydrofluoric acid to fully cleave RNA into mono-nucleosides, thereby minimizing the search space to drastically enhance coverage and to reach single amino acid resolution. The simple mono-nucleoside adducts offer a confident and quantitative measure of direct RNA-protein interaction. Using RBS-ID, we profiled ~2,000 human RBSs and probed *Streptococcus pyogenes* Cas9 to discover residues important for genome editing. I also introduce formaldehyde crosslinking (FAX) as an alternative chemical crosslinking for RNA interactome capture (RIC). Mild FAX captures RNA-protein interaction with high specificity and efficiency in cell culture. Furthermore, FAX-RIC is applicable to mammalian tissue samples such as *Mus musculus* liver, extending the RNA interactome profiling into multicellular organisms.

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

Emerging International Organic Chemists

Room 304 (Live Streaming) THU 10:50

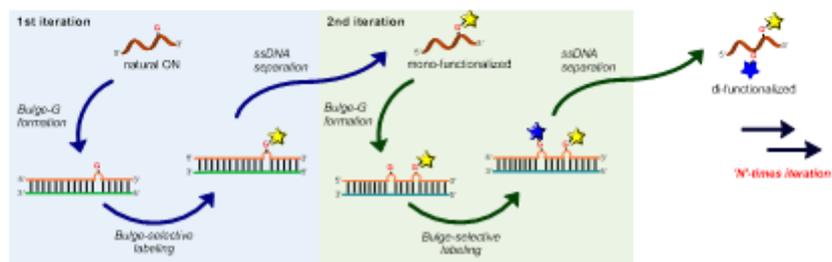
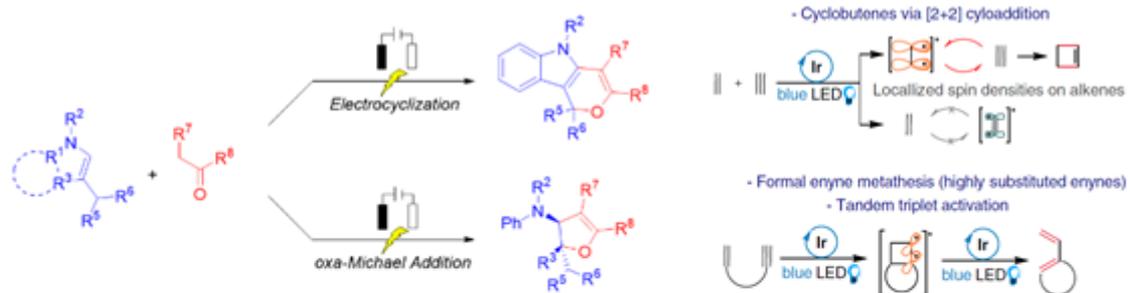
Chair: Eun Joo Kang (Kyung Hee University)

Reactive Intermediates in Organic Synthesis : from Small to Macro Molecules

Cheol-Min Park

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

Heterocycles are among the most significant structural components of pharmaceuticals. Among the unique small-molecule drugs in U.S. FDA database, nearly 60% contains at least one N-heterocycle. N-Heterocycles possess essential properties including hydrogen bonding interactions and favorable physicochemical properties. Given the composition, frequency, and structural diversity in drug molecules, development of efficient synthetic methods for N-heterocycles is highly important. In this talk, several approaches for the synthesis of heterocycles will be discussed. Reactive intermediates including carbenes and radicals serve as powerful tools for bond formation. To access these reactive species, we have explored the reactivity of transition metal catalysts, photocatalysts, and electrolysis, which led to the discovery of unique annulation reactions that allowed the synthesis of various heterocycles. Considerable efforts have been made to establish the mechanistic understanding in depth. Moreover, we were able to extend the synthetic methodology toward the modification of biomolecules, and the details on the development of site-selective post-synthetic labeling of oligonucleotides will be discussed. References Choi, S.; Park, J.; Yu, E.; Sim, J.; Park, C.-M. Electrosynthesis of Dihydropyrano[4,3-b]indoles Based on a Double Oxidative [3+3] Cycloaddition. *Angew. Chem. Int. Ed.* 2020, 59, 11886. Ha, S.; Lee, Y.; Kwak, Y.; Mishra, A.; Yu, E.; Ryou, B.; Park, C.-M. Alkyne–Alkene [2 + 2] cycloaddition based on visible light photocatalysis. *Nature Commun.* 2020, 11, 2509. Lee, Y.; Yu, E.; Park, C.-M. Programmable Site-selective Labeling of Oligonucleotides Based on Carbene Catalysis. *Nature Commun.* 2021, in press.



Symposium : **ORG1-1**

Emerging International Organic Chemists

Room 304 (Live Streaming) THU 09:00

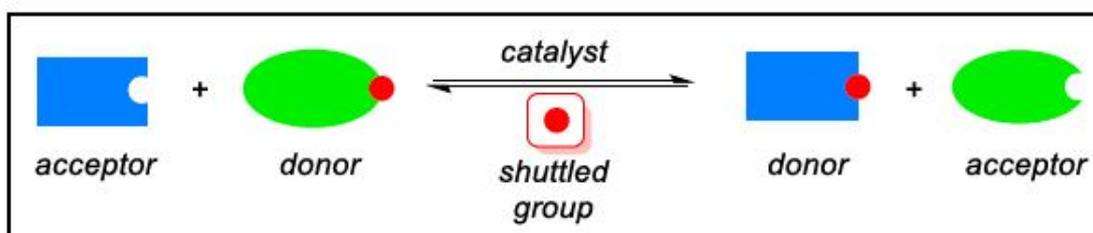
Chair: Sunkyu Han (KAIST)

Recent developments in shuttle catalysis

Bill Morandi

Chemistry & Applied Biosciences, ETH Zurich, Switzerland

Catalytic reversible reactions, such as alkene metathesis and transfer hydrogenation, have had an auspicious impact on the molecular sciences. This presentation will describe our recent efforts to develop related “shuttle catalysis” reactions for the functionalization and defunctionalization of organic compounds. These reactions avoid the use of toxic reagents (e.g. Cl₂, CO) through the reversible transfer of chemical moieties between organic molecules. Due to their reversibility, these reactions can also be employed for the recycling of end-of-life chemicals, such as pest-control agents. Shuttle catalysis has further been employed in the development of novel C–X bond metathesis reactions that can help to address significant synthetic challenges across the molecular sciences, most notably in the area of materials science.



Symposium : **ORGN1-2**

Emerging International Organic Chemists

Room 304 (Live Streaming) THU 09:30

Chair: Sunkyu Han (KAIST)

Photoenzymatic Catalysis – Using Light to Reveal New Enzyme Functions

Todd Hyster

Department of Chemistry and Chemical Biology, Cornell University, United States

Enzymes are exquisite catalysts for chemical synthesis, capable of providing unparalleled levels of chemo-, regio-, diastereo- and enantioselectivity. Unfortunately, biocatalysts are often limited to the reactivity patterns found in nature. In this talk, I will share my groups efforts to use light to expand the reactivity profile of enzymes. In our studies, we have exploited the photoexcited state of common biological cofactors, such as NADH and FMN to facilitate electron transfer to substrates bound within enzyme active sites. In other studies, we found that enzymes will electronically activate bound substrates for electron transfer. In the presence of common photoredox catalysts, this activation can be used to direct radical formation to enzyme active sites. Using these approaches, we are able to develop biocatalysts to solve long-standing selectivity challenges in chemical synthesis.



Symposium : **ORGN1-3**

Emerging International Organic Chemists

Room 304 (Live Streaming) THU 10:00

Chair: Sunkyu Han (KAIST)

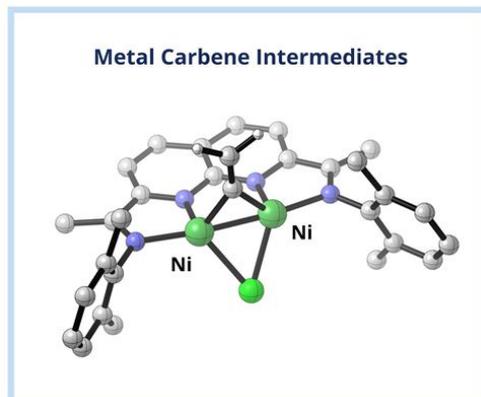
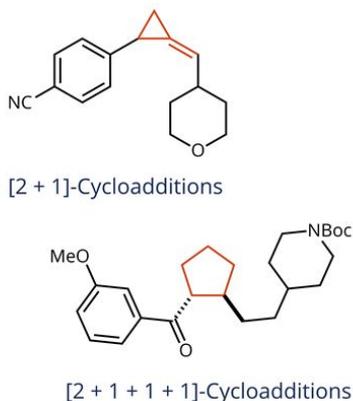
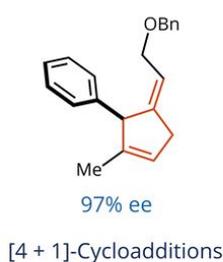
The Simmons–Smith Reaction in the Age of Catalysis

Christopher Uyeda

Department of Chemistry, Purdue University, United States

Carbenes are versatile reactive intermediates that display orthogonal reactivity to common nucleophilic and electrophilic functional groups. Homogeneously catalyzed carbene transfer reactions were first discovered over a half century ago, and numerous examples of $[n + 1]$ -cycloaddition reactions have now been developed, often with control over diastereo- and enantioselectivity. Nearly all of these reactions rely on the controlled decomposition of diazoalkane precursors as a central strategy for accessing reactive carbene equivalents. Despite the utility of diazoalkanes in organic synthesis, they are inherently limited by the need for stabilizing substituents such as aryl or carbonyl groups. In order to develop transfer reactions of non-stabilized carbenes, such as methylene, isopropylidene, and vinylidene, it would be necessary to identify an alternative set of precursors. Our group has shown that nickel and cobalt catalysts can promote reductive $[n + 1]$ -cycloaddition reactions using readily available and indefinitely stable 1,1-dichloroalkanes and 1,1-dichloroalkenes as carbene precursors. In this seminar, I will describe our development of new cycloaddition methods and our current hypotheses about the mechanisms of these reactions.

Cycloaddition Reactions



Symposium : **ORGN2-1**

Current Trends in Chemical Synthesis

Room 304 (Live Streaming) THU 13:00

Chair: Sang Kook Woo (University of Ulsan)

Umpolung Chemistry Enabled by N-O Bond Redox via Polar or Radical Mechanisms

Seunghoon Shin

Department of Chemistry, Hanyang University, Korea

N-O bond-containing oxidation has several advantageous aspects. They are relatively weak, and once appropriately incorporated into the organic substrates, they mediate efficient yet selective oxidation. In addition, they are functionally diverse, allowing for a wide spectrum of reactivity that is modulated by different classes of catalysts. Three different catalytic systems could be envisioned for the interaction of N-O oxidants with alkynes: (1) gold catalysis,¹ (2) Brønsted acid catalysis,² (3) visible-light photoredox catalysis. In this presentation, our recent progress on the last two aspects will be discussed. References 1. Yeom, H. -S.; Shin, S. Catalytic Access to α -Oxo Gold Carbenes by N-O Bond Oxidants, *Acc. Chem. Res.* 2014, 47, 9662. Patil, D. V.; Shin, S. Organocatalytic Oxidative Functionalization of Alkynes, *Asian J. Org. Chem.* 2019, 8, 63.

Symposium : **ORGN2-2**

Current Trends in Chemical Synthesis

Room 304 (Live Streaming) THU 13:20

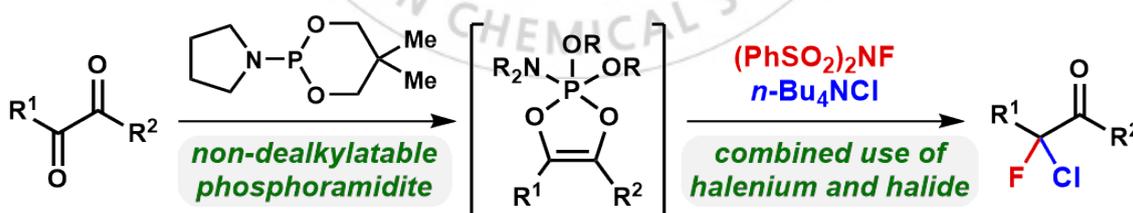
Chair: Sang Kook Woo (University of Ulsan)

Phosphorus(III)-Mediated, Tandem Deoxygenative Geminal Chlorofluorination of 1,2-Diketones

Won-jin Chung

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

We have developed an efficient synthetic method that gives access to a tetrasubstituted carbon center with two different halogen substituents in a single-step operation. The newly designed phosphoramidite allows the formation of non-dealkylatable dioxaphospholene as a suitable carbene surrogate for the combined use of electrophilic halenium and nucleophilic halide. The current method is applicable to a variety of aryl-aryl as well as aryl-cyclopropyl 1,2-diketones albeit the moderate site selectivity for unsymmetrical substrates. The structure of geminal chlorofluoride was unambiguously established by X-ray crystallographic analysis. In addition, the more reactive chlorine substituent could be selectively functionalized to give a tertiary alkyl fluoride. (Choi, G.; Kim, H. E.; Hwang, S.; Jang, H.; Chung, W.-j. *Org. Lett.* **2020**, 22, 4190–4195.)



- dioxaphospholene as carbene surrogate
- tandem, one-step gem-chlorofluorination
- no halogen scrambling

Symposium : **ORGN2-3**

Current Trends in Chemical Synthesis

Room 304 (Live Streaming) THU 13:40

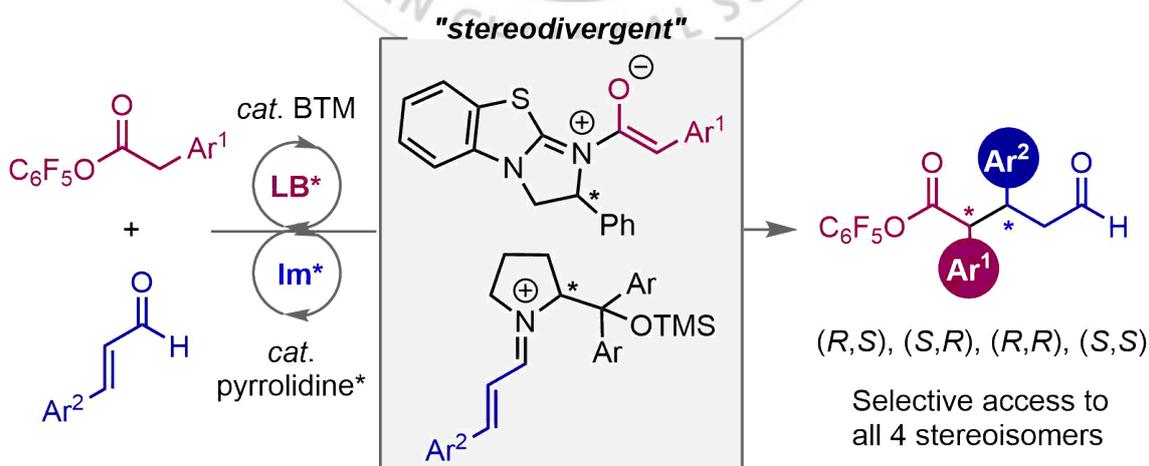
Chair: Sang Kook Woo (University of Ulsan)

Stereodivergent Carbon-Carbon Bond Formation by Synergistic Organocatalysis

Sarah Yunmi Lee

Department of Chemistry, Yonsei University, Korea

The control of stereoselectivity has been one of the central goals in synthetic organic chemistry due to the presence of chiral molecules in a wide range of natural products and pharmaceuticals. Despite remarkable advances in asymmetric synthesis, the development of catalyst-controlled processes that precisely control relative and absolute configurations of multiple stereocenters is a persistent challenge. In this seminar, I describe a method for the stereodivergent carbon-carbon bond formation catalyzed synergistically by two chiral organocatalysts that furnishes 1,5-aldehydes esters containing two adjacent stereocenters. By altering the relative chirality of catalyst combinations, all four stereoisomers of the products are accessible with high enantio- and diastereoselectivity.



Symposium : **ORGN2-4**

Current Trends in Chemical Synthesis

Room 304 (Live Streaming) THU 14:10

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

Development of β -Lactam-Based Chemical Probes for Detection of Antibiotic Resistant Bacteria

Sun-Joon Min

Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea

The emergence of antibiotic-resistant bacteria has been a serious threat to the public health. A primary mechanism of the drug resistance is involved in expression of β -lactamases (Blas), a group of enzymes, which can specifically hydrolyze the amide bond of the β -lactam antibiotics, resulting in loss of the antibiotic activity. Several cases of therapeutic failure have been reported due to the poor susceptibility of β -lactamase inhibitors and rapid transmission of such enzyme by plasmid. Accordingly, development of efficient and accurate detection method of β -lactam-resistant bacteria is required for infection control and guidance. Current detection methods of β -lactamase producing bacteria can be categorized into phenotypic and genotypic methods. The genotypic methods based on molecular diagnostics are accurate but they can detect only the genes of which sequence is known. Alternatively, many phenotypic methods have been reported. However, they are still time-consuming and lack of sensitivity and specificity. Most recently, activity-based detection methods have been developed to overcome these disadvantages. In particular, fluorescence-based assays are attractive owing to relatively low cost, high sensitivity and operational simplicity. In this study, we report synthesis and evaluation of novel fluorogenic β -lactamase substrates for the specific detection of the β -lactamase-producing antibiotic resistant bacteria. These probes consist of β -lactam core scaffolds, appropriate linker and fluorescence dyes, which can turn on fluorescence signal upon hydrolysis by β -lactamases. The result from clinical assessment of our probes indicated that they would provide practical screening tools for rapid and accurate detection of the antibiotic resistant bacteria.

Symposium : **ORGN2-5**

Current Trends in Chemical Synthesis

Room 304 (Live Streaming) THU 14:30

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

Molecular Design Strategy of the Efficient Generation of Reactive Oxygen Species and Their Protein Dysfunction Mechanism for Photodynamic Therapy

Tae-Hyuk Kwon

Chemistry, Ulsan National Institute of Science and Technology, Korea

Reactive oxygen species (ROS, 1O_2 , $O_2^{\cdot-}$, OH^{\cdot} , and H_2O_2) has known as one of the very important factors for biomedical applications, such as phototherapeutics for non-invasive therapy (photodynamic therapy; PDT) and wound healing hemostasis for fast cell recovery from serious injury or surgery. The controlling and understanding of ROS give insight into the clue of cell death mechanism or cell recovery by ROS, which will be helpful to overcome the chronic or pathogenic diseases like cancer or Alzheimer as well as aging. Until now, Ir(III) complexes have known as an efficient PDT photosensitizer because of their (i) high photostability, (ii) efficient triplet state utilization followed by (iii) high 1O_2 quantum yield in aqueous media, and (iv) preference of hypoxia condition. However, there is no detailed molecular design strategy of ROS generation and the understanding of cell death mechanism by ROS. For this aim, our group have investigated on the Ir(III) complex based photosensitizers as well as organelle probes for the understanding of the interaction between proteins during the cell death. In this presentation, Ir(III) complexes based molecular design strategy will be presented for efficient ROS generation and their cell death mechanism based on proteomic analyses and phenomenological observations. In addition, we introduce a new 1O_2 generator based on an aliphatic polyaminoglycerol (PAG), which relies on spin-flip electron transfer.

Symposium : **ORGN2-6**

Current Trends in Chemical Synthesis

Room 304 (Live Streaming) THU 14:50

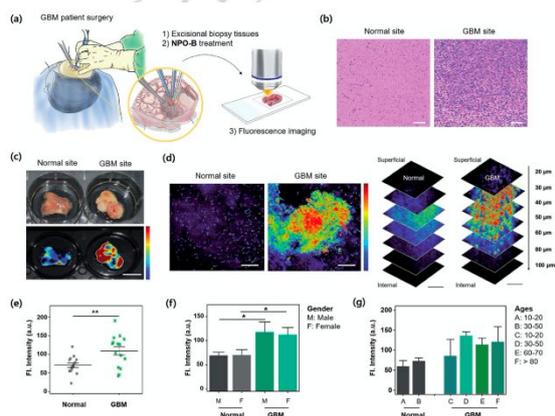
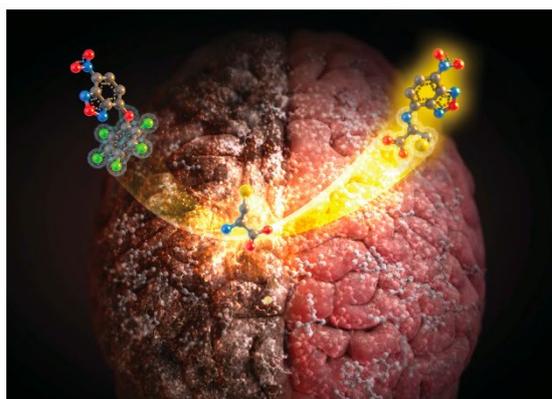
Chair: Min Hee Lee (Sookmyung Women's University)

Development of Fluorescent Probes for Visualization of Human Glioblastoma

Dokyoung Kim

College of Medicine, Kyung Hee University, Korea

Glioblastoma is the most aggressive form of cancer that originates within the central nervous system. Generally, glioblastoma's clinical management has been reliant on neurological assessment and clinical imaging techniques, including magnetic resonance imaging, computed tomography, positron emission tomography, and biopsy sampling. In this presentation, the author will introduce new approaches to develop fluorescent probes to visualize human glioblastoma that could be applicable for image-guided surgery. [First example] A Smiles rearrangement inspired cysteine-selective fluorescent probe. [Second example] Triple receptor-targeting fluorescent complex.



Symposium : **MEDI-1**

The Cutting Edge of Medicinal Chemistry

Room 306 (Live Streaming) THU 10:00

Chair: Jungwook Chin (DGMIF)

DISCOVERY OF A POTENT ERK INHIBITOR FOR THE TREATMENT OF ADVANCED SOLID TUMORS HARBORING MAPK PATHWAY ALTERATIONS

Wooseok Han

R&D Center, Cyrus Therapeutics, United States

The mitogen activated protein kinase (MAPK) pathway is a key signaling cascade that drives cell proliferation, differentiation, and survival. Genetic alterations at multiple nodes in this pathway, e.g. RAS and BRAF mutations, are a common feature in human cancers, thereby leading to activated ERK signaling to drive oncogenesis. Inhibitors against BRAF or MEK have demonstrated efficacy in clinical trials via suppression of MAPK pathway. However, these effects are short-lived due to multiple acquired resistance mechanisms which commonly reactivate ERK1/2 signaling. In this setting, inhibition of ERK1/2, which are the most distal kinases in the MAPK signaling cascade, could effectively inhibit MAPK signaling, resulting in anti-tumor effects. Herein, we present the medicinal chemistry approaches which led to the discovery of a potent and orally bioavailable small molecule inhibitor of ERK1/2. It has shown efficacy in a wide range of MAPK pathway-driven human cancer cell lines and in vivo tumor xenografts and is being tested in a Phase 1 trials as a single agent and in combination with a b/c-RAF inhibitor.

Symposium : **MEDI-2**

The Cutting Edge of Medicinal Chemistry

Room 306 (Live Streaming) THU 10:30

Chair: Jungwook Chin (DGMIF)

Discovery of ORIC-101, a Potent and Selective Steroidal Glucocorticoid Receptor in Clinical Development

Yosup Rew

IntoCell, Korea

The glucocorticoid receptor (GR) is a member of the nuclear receptor superfamily, which is activated by its endogenous steroid hormone ligand cortisol, and by synthetic glucocorticoid agonists such as dexamethasone. Numerous preclinical studies have revealed that GR mediates resistance to both targeted cancer therapies and cytotoxic chemotherapies in a variety of epithelial cancers including prostate, lung, bladder, renal, ovarian and triple-negative breast cancers. These findings suggest that targeted cancer therapies or cytotoxic chemotherapies in combination with a GR antagonist could be a more efficacious approach to cancer treatment. The presentation will describe the SAR efforts toward finding selective GR antagonists. Lead optimization starting with mifepristone and employment of structure-based drug design led to the discovery of ORIC-101, a highly potent steroidal GR antagonist with reduced AR agonistic activity and lower CYP inhibition relative to mifepristone. Moreover, ORIC-101 has an excellent pharmacokinetic profile and demonstrated in vivo antitumor activity in a chemo-resistant OVCAR5 ovarian cancer xenograft model. ORIC-101 is currently being evaluated in two separate Phase 1b trials in combination with: (1) Xtandi (enzalutamide) in metastatic prostate cancer and (2) Abraxane (nab-paclitaxel) in advanced or metastatic solid tumors.

Symposium : **MEDI-3**

The Cutting Edge of Medicinal Chemistry

Room 306 (Live Streaming) THU 11:00

Chair: Jungwook Chin (DGMIF)

Discovery and SAR studies of gingerol analogs as biofilm inhibitors of *Pseudomonas aeruginosa*

Youngjoo Byun

Department of Pharmacy, Korea University, Korea

The National Institutes of Health reported that more than 80% of microbial infections are associated with biofilm formation. Biofilms are closely associated with lung and urethral infections, burns, cystic fibrosis, pneumonia, or sepsis. The opportunistic human pathogen *Pseudomonas aeruginosa* (*P. aeruginosa*) is the leading cause of death in patients with cystic fibrosis. Quorum sensing (QS) is a bacterial cell-cell communication system that regulates group behaviors such as biofilm formation and virulence factor production. Therefore, controlling *Pseudomonas aeruginosa*'s QS system can be a new antibiotic strategy that inhibits biofilm formation and virulence factor production of *P. aeruginosa*. We screened ginger ingredients and identified 6-gingerol as a potential LasR inhibitor¹ and 4-gingerol as a RhlR inhibitor, respectively. As LasR and RhlR are key transcriptional regulators in the QS mechanism in *P. aeruginosa*, they are attractive target proteins for attenuating biofilm formation. As an attempt to discover new biofilm inhibitors targeting LasR or RhlR, we synthesized and evaluated a series of new gingerol-derived analogs. Structure-activity relationship (SAR) studies showed that hydrogen-bonding interactions in the head section, stereochemistry and rotational rigidity in the middle section, and alkyl chain length in the tail section of gingerol are important factors for inhibiting LasR and RhlR activities as well as the inhibition of biofilm formation. (R)-8-gingerol analog with restricted rotation exhibited the strongest LasR-inhibitory activity while 4-gingerol analog substituted with fluoro groups in the head section and the alkynyl ketone group in the middle section was identified as the most potent RhlR antagonist. References 1. H Choi, SY Ham, E Cha, HS Kim, JK Bang, SH Son, HD Park*, Y Byun*, Structure-activity relationships of 6- and 8-gingerol analogs as anti-biofilm agents, *Journal of Medicinal Chemistry*, 2017, 60(23), 9821-9837. SJ Nam, S-Y Ham, H Kwon, H-S Kim, S Moon, J-H Lee, T Lim, S-H Son, H-D Park*, Y Byun*, Discovery and Characterization of Pure RhlR Antagonists against *Pseudomonas aeruginosa* Infections, *Journal of Medicinal Chemistry*, 2020, 63(15), 8388-8407

Symposium : **MEDI-4**

The Cutting Edge of Medicinal Chemistry

Room 306 (Live Streaming) THU 11:30

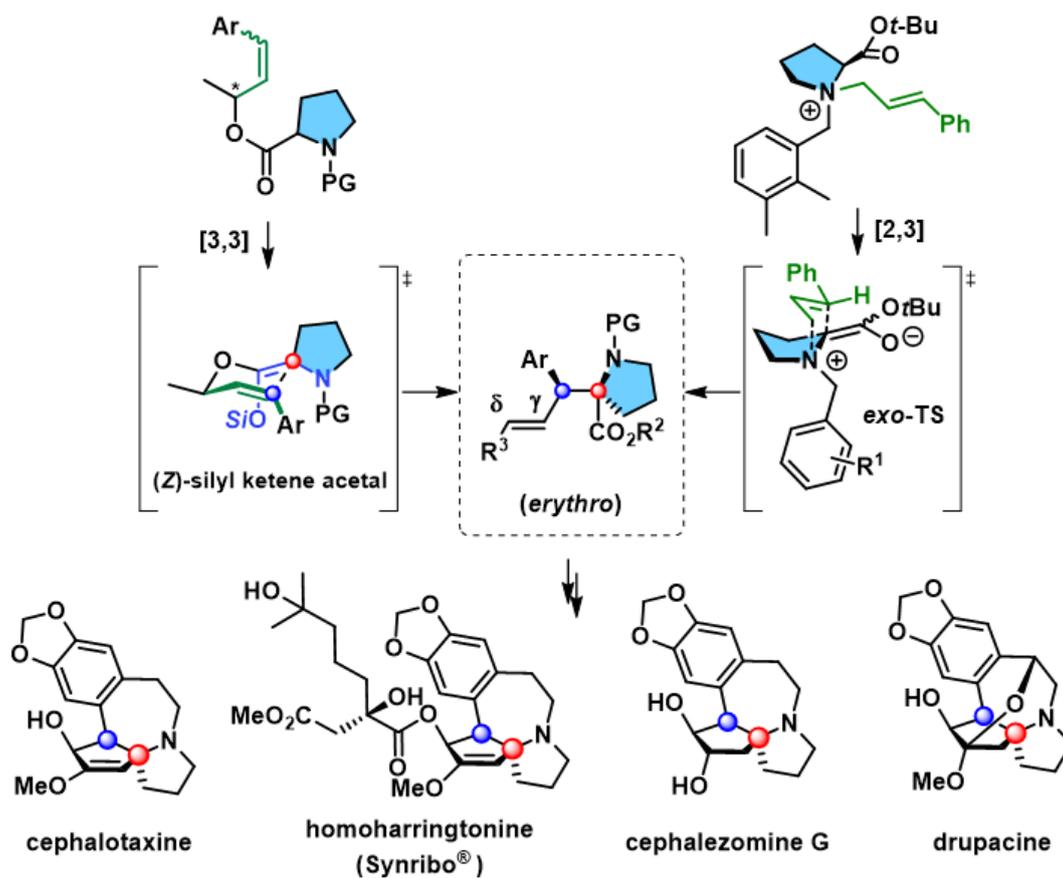
Chair: Jungwook Chin (DGMIF)

Rearrangement of Proline Derivatives in the Total Synthesis of *Cephalotaxus* Alkaloids

Hongjun Jeon

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

Proline derivatives, particularly α -substituted proline derivatives, have been recognized as very attractive substances due to their wide range of applicability in chemistry and biology. A number of strategies for the asymmetric synthesis of α -substituted proline derivatives have been devised. One of the promising and effective strategy would be [i,j]-sigmatropic rearrangement, from which enantioenriched proline derivatives are readily accessed by its well-defined transition state conformation. Using these rearrangements as a key strategy, such as [3,3]-ester enolate–Claisen rearrangement and [2,3]-Stevens rearrangement, several *Cephalotaxus* alkaloids have been synthesized. Notably, each rearrangement strategy has been applied to the total synthesis in concert with the concept of a nonplanarity of *o*-substituted styrene moiety and C to N to C chirality transfer, respectively.



Symposium : **MAT1-1**

Catalytic Applications of Inorganic Nanohybrid Materials

Room 405 (Live Streaming) THU 10:20

Chair: Hyojong Yoo (Hanyang University)

Highly Durable PEMFC Catalysts Using Polymer-Based Carbon Supports with Ultralow Pt Loadings

Hyunjoo Lee

Department of Chemical Engineering & Biotechnology, Korea Advanced Institute of Science and Technology, Korea

Minimizing the use of Pt catalysts in proton exchange membrane fuel cells (PEMFC) is important, considering its high price and scarcity. Herein, we demonstrate novel catalysts for PEMFCs with exceptionally high mass activity and durability, in which block copolymer-based carbon supports are loaded with an ultra-small amount of Pt. The mass activity measured after 30,000 cycles of single cell tests was 0.81 A mg⁻¹Pt at 0.9 V, which is the highest performance reported to date. The newly developed catalyst yielded nearly the same power density as that of the commercial Pt/C, even with 1/20 of Pt usage. The carbon supports were prepared by carbonizing crosslinked domain of block copolymer particles selectively, resulting in mesoporous carbon particles with ~25 nm pores. When Pt was deposited, thin carbon shells were formed encapsulating PtFe nanoparticles, catalyzing oxygen reduction reaction efficiently with high durability.

Symposium : **MAT1-2**

Catalytic Applications of Inorganic Nanohybrid Materials

Room 405 (Live Streaming) THU 10:45

Chair: Hyojong Yoo (Hanyang University)

Design of Interface-Confined High-Performance Pt-Single Atoms

Hyunyou Kim

Materials Science and Engineering, Chungnam National University, Korea

Utilizing Pt single-atoms as a reaction site resolves a grand challenge in the economic use of Pt in catalysis. By manipulating the chemical nature of multi-component interfaces, we demonstrate a strategy for controlled formation of highly reactive CO-tolerant Pt single-atom catalysts activated at CeO₂-TiO₂ interfaces. The addition of Ce to TiO₂ support particles creates a CeO₂-TiO₂ interface, resulting in a strong electronic interaction between Pt and CeO₂-TiO₂ interfaces that stabilizes Pt single-atoms. We identify how the CeO₂-TiO₂ interfaces activate the interface-mediated Mars-van Krevelen mechanism of CO oxidation, protecting Pt single-atoms from CO-poisoning. Addition of 1 wt.% Ce enhances the CO oxidation activity relative to a bare Pt/TiO₂ catalyst by a factor of 15.1 and improved the long-term stability of Pt-single atoms under the harsh reaction conditions. These results elaborate how the noble metal single-atom catalysts can be generated and optimized by atomic-scale tuning of the metal-support interface.

Symposium : **MAT1-3**

Catalytic Applications of Inorganic Nanohybrid Materials

Room 405 (Live Streaming) THU 11:10

Chair: Hyojong Yoo (Hanyang University)

Photoelectrochemical H₂O Oxidative H₂O₂ Synthesis

Jong hyeok Park

Department of Chemical and Biomolecular Engineering, Yonsei University, Korea

Here, we report a SnO₂-x overlayer coated BiVO₄ photoanode, which demonstrates a great ability to near-completely suppress O₂ evolution for photoelectrochemical (PEC) H₂O oxidative H₂O₂ evolution. Based on the surface hole accumulation measured by surface photovoltage, downward quasi-hole Fermi energy at the photoanode/electrolyte interface and thermodynamic Gibbs free energy between 2-electron and 4-electron competitive reactions, we are able to consider the photoinduced holes of BiVO₄ that migrate to the SnO₂-x overlayer kinetically favour H₂O₂ evolution with great selectivity by reduced band bending. The formation of H₂O₂ may be mediated by the formation of hydroxyl radicals (OH•), from 1-electron water oxidation reactions, as evidenced by spin-trapping electron paramagnetic resonance (EPR) studies conducted herein. In addition to the H₂O oxidative H₂O₂ evolution from PEC water splitting, the SnO₂-x/BiVO₄ photoanode can also inhibit H₂O₂ decomposition into O₂ under either electrocatalysis or photocatalysis conditions for continuous H₂O₂ accumulation. Overall, the SnO₂-x/BiVO₄ photoanode achieves a Faraday efficiency (FE) of over 86% for H₂O₂ generation in a wide potential region (0.6~2.1 V vs. reversible hydrogen electrode (RHE)) and an H₂O₂ evolution rate averaging 0.825 μmol/min/cm² at 1.23 V vs. RHE under AM 1.5 illumination, corresponding to a solar to H₂O₂ efficiency of ~5.6%; this performance surpasses almost all previous solar energy-assisted H₂O₂ evolution performances. Because of the simultaneous production of H₂O₂ and H₂ by solar water splitting in the PEC cells, our results highlight a potentially greener and more cost-effective approach for “solar-to-fuel” conversion.

Symposium : **MAT1-4**

Catalytic Applications of Inorganic Nanohybrid Materials

Room 405 (Live Streaming) THU 11:35

Chair: Hyojong Yoo (Hanyang University)

Hollow Nanoreactors as Catalytic Platform for Bioorthogonal Synthesis in Living Systems

In Su Lee

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

Synthetic nanoreactors, capable of achieving speedy bioorthogonal catalytic transformations on-demand despite of the highly complex bio-environment and uncontrollable reaction conditions, have great significance in biomedical science and chemical biology. But, such bio-applicable catalytic platforms, where rate of the reactions can be remotely induced and controlled, have been little synthesized and applied. In this talk, I will present our recent efforts to design and synthesize catalytic hollow nanoreactors for promoting organic reactions in complex bio-media and living cells, using a remotely operable magnetic field- or light-induced effects. As the key synthetic strategy for catalytic nanoreactors, we could functionalize interior space and surfaces of hollow silica nanoparticles in spatio-specific manner, by adopting the nanospace-confined reaction approach that has been pursued by our group over the years. Owing to the synergy between localized thermal-effects and catalytic activities of functional nanocrystals, integrated within a protected and confined nanosized space, the developed hollow nanoreactors could efficiently and selectively affect the transformation of small-sized organic molecules in physiologically relevant complex conditions and, moreover, remotely control the bioorthogonal catalytic synthesis in living cells with highly accelerated reaction rates. I will also discuss our research directions towards versatile and adaptable method for efficient activation of diverse catalytic reactions inside living systems and expanding the scope towards the development of new and versatile bioorthogonal chemistry-methodologies.

Symposium : **MAT2-1**

Advanced electrocatalytic materials for clean energy and chemical feedstocks

Room 405 (Live Streaming) THU 13:00

Chair: Jin Young Kim (KIST)

Electrochemical Interface Design for Carbon Dioxide Conversion

Youngkook Kwon

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

Electrochemical conversion of CO₂ to fuels or stock chemicals with high-energy density would be a major step forward in the introduction of a carbon neutral energy cycle. One of the achievements in electrochemical CO₂ reduction is the clarification of the catalysts toward two-electron involved products such as CO and formate. Interestingly, CO/formate ratio can be selectively controlled on formate selective catalyst such as Sn by tuning the interfacial electric field. On the other hand, on copper catalyst, the selection of alkali cations has direct influence on activity and product selectivity; increasing the size of mono-valent cations can increase the activity and selectivity toward C-C coupled products by modulating the interaction energy between adsorbates and electric fields at the interface. In addition, copper catalyst with a specific atomic-scale gap accelerates the reaction kinetics and selectivity to C₂+ products. Therefore, understanding the roles of catalyst, support and electrolyte offers the design of efficient, yet cheap electrochemical CO₂ reduction systems.

Symposium : **MAT2-2**

Advanced electrocatalytic materials for clean energy and chemical feedstocks

Room 405 (Live Streaming) THU 13:25

Chair: Jin Young Kim (KIST)

(Photo)Electrocatalytic Water Splitting for Production of Value-Added Chemicals

Hyunwoong Park

School of Energy Engineering, Kyungpook National University, Korea

The global demand for clean, cheap, and sustainable energy resources is tremendously escalating and is driven by technological advancements. The most promising source of renewable and clean energy is solar power. There are several types of photosystems, including photocatalysis, photoelectrocatalysis, and photovoltaic-assisted electrocatalysis. Among them, the last has been considered the most promising due to the easy fabrication, high efficiency, and scalability, while the formers are still actively developed. The photosystem-based water splitting has received long attention as a viable process for HER and CO₂RR while evolving O₂ from water in a single device. Many non-noble metal-based HER/CO₂RR electrocatalysis have been developed. Several CO₂ conversion products (C1-C6) are possible, while formate and CO are considered one of the most-cost effective. The other 2-electron transfer water oxidation and ORR can be designed for the production of H₂O₂. This talk will briefly summarize the photosystems in terms of efficiency, durability, and mechanism, and discuss the hybrid systems that split various types of water while driving OER, ORR, HER, and CO₂RR.

Symposium : **MAT2-3**

Advanced electrocatalytic materials for clean energy and chemical feedstocks

Room 405 (Live Streaming) THU 14:00

Chair: Jin Young Kim (KIST)

Phase Engineering in Transition Metal Dichalcogenides Toward Efficient Electrocatalysis

Hyesung Park

Department of Materials Science and Engineering, UNIST, Korea

Developing efficient bifunctional catalysts for overall water splitting that are earth-abundant, cost-effective, and durable is of considerable importance from the practical perspective to mitigate the issues associated with precious metal-based catalysts. In the present study, we introduce two different types of heterostructures comprising perovskite oxides and transition metal dichalcogenides as the electrochemical catalyst for overall water electrolysis. First, in a heterostructure comprising $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_{3-\delta}$ (LSC) and 2H-phase molybdenum diselenide (MoSe_2), a local phase transition in MoSe_2 , 2H to 1T phase, was induced owing to the electron transfer from Co to Mo, which significantly enhanced the electrochemical activities of the heterostructure for both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). In the overall water splitting operation, the heterostructure showed excellent stability at a high current density of 100 mA cm^{-2} over 1,000 h, which is exceptionally better than the stability of the state-of-the-art Pt/C || IrO_2 couple. Second, we introduce a facile and scalable synthesis of 1T-phase transition metal dichalcogenides (TMDs) via the molten metal-assisted intercalation (MMI) approach, which exploits the capillary action of molten potassium and the difference between the electron affinity of TMDs and the ionization potential of potassium. A heterostructure comprising LSC and 1T-phase MoSe_2 prepared via MMI (LSC&1T- MoSe_2 (MMI)) showed much improved HER and OER activities than the LSC and 1T- MoSe_2 (MMI). The performance improvement is attributed to decreased charge transfer resistance, improved active surface area, increased hydrogen/oxygen adsorption capability, and improved exchange current density in the heterostructure. We hypothesize that bidirectional electron transfer from LSC to MoSe_2 and from potassium to MoSe_2 improves 1) HER performance via electron-rich MoSe_2 with high electrical conductivity and 2) OER performance by increasing the electrophilicity of LSC. In the overall water electrolysis, the heterostructure (LSC&1T- MoSe_2 (MMI) || LSC&1T- MoSe_2 (MMI)) showed excellent chronopotentiometric stability over the state-of-the-art Pt/C || IrO_2 couple.

Symposium : **MAT2-4**

Advanced electrocatalytic materials for clean energy and chemical feedstocks

Room 405 (Live Streaming) THU 14:25

Chair: Jin Young Kim (KIST)

Novel Insights into Lithium-ion Storage Behaviors of Mesoporous Electrode Materials

Ji Man Kim

Department of Chemistry, Sungkyunkwan University, Korea

Nanostructured materials have a potential to make a considerable impact on the lithium-storage performances including energy density, power density and cycle life. We demonstrate mesoporous metal oxide materials with abnormal lithium storage site, which exhibit the reversible capacities that exceed their theoretical capacity based on the conversion and/or alloy reaction. Contrary to previous reports, we provide insights into the electrochemical results, obtained by in situ X-ray absorption, in situ X-ray scattering, scanning transmission electron microscopy analysis, indicating that the nano-scale pore engineering of transition metal oxides enables an unexpected electrochemical mass storage reaction mechanism. This finding, which is unveiling lithium storage reaction mechanism with extraordinary lithium storage capacity, not only provides an opportunity to understand further the unusual results of nano-electrodes on the lithium storage process but also emphasizes that the design of novel nanostructured material enables an unexpected electrochemical mass storage reaction opening the advances up for next generation lithium ion batteries.

Symposium : **MAT3-1**

Recent Trends in Infrared Nanomaterials

Room 405 (Live Streaming) THU 15:10

Chair: Kwang Seob Jeong (Korea University)

Synthesis and Surface Engineering of III-V Semiconductor Quantum Dots for Infrared Optoelectronic Applications

Nuri Oh

Division of Materials Science and Engineering, Hanyang University, United States

Colloidal quantum dots (QDs) have widely been considered as emerging candidates for solution-processable optoelectronic devices. Especially, QDs that are optically active in NIR and SWIR spectral windows, offer a great promise for infrared emitters, infrared photodetectors, photovoltaics, and biological imaging applications. It is thus essential to develop high-quality infrared QDs without the use of heavy metals such as cadmium, lead, or mercury. Among various semiconducting materials, III-V compound semiconductors show great potential in practical optoelectronic applications not only due to their wide tunability in the infrared region, but also due to their excellent optical and electronic properties. However, the synthesis of III-V semiconductor-based QDs has been limited by the lack of understanding about the precursors of group V elements such as P, As and Sb. In this presentation, we would like to discuss about the pnictogen precursors to synthesize various III-V QDs and also the surface properties of the resultant QDs. By controlling the reaction process with the pnictogen precursors, we achieve size and stoichiometry-tunable III-V QDs including InAs, InSb QDs. Based on structural, analytical, optical, and electrical characterization of the QDs, we study the effects of surface treatments on their optoelectronic properties. We demonstrate that III-V QD thin films are promising candidate materials for infrared optoelectronic devices.

Symposium : **MAT3-2**

Recent Trends in Infrared Nanomaterials

Room 405 (Live Streaming) THU 15:35

Chair: Kwang Seob Jeong (Korea University)

Energy-level tuned quantum dot solids for efficient optoelectronics

Sohee Jeong

Department of Energy Science, Sungkyunkwan University, Korea

Colloidal quantum dots are nano-sized semiconductors which exhibit unique size-dependent optoelectronic properties dictated by the quantum confinement effect. The true benefit of such unique quantum size effects depends on the ability to synthesize QDs of a wide range of sizes with a narrow size distribution at high reaction yield. While an adjustable band gap of colloidal quantum dots promises an efficient harvesting of near-IR solar spectrum when used in photovoltaics, tunability in band edge position of quantum dots draws immense attention as the energy level of semiconductor determine their functionality in various optoelectronic applications including photovoltaics. Here we discuss that the band edge position of lead sulfide colloidal quantum dots can be controlled upto 2 eV by careful design of molecules or atoms on nanocrystal surfaces based on atomistic understanding of surface structure. Further by modulating bandgap and band edge position of quantum dot solids, we demonstrate that the indium arsenide quantum dot solids can serve as a stable n-type layers for quantum dot photovoltaics or electron transport layer for efficient and stable organic photovoltaics.

Symposium : **MAT3-3**

Recent Trends in Infrared Nanomaterials

Room 405 (Live Streaming) THU 16:10

Chair: Kwang Seob Jeong (Korea University)

Surface Chemistry of Infrared Ag₂S Nanocrystals

Sung Jee Kim

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

The surface stoichiometry of colloidal Ag₂S nanocrystals (NCs) is rigorously controlled. Ag₂S NCs with Ag-rich surface (Ag-Ag₂S) and Ag₂S NCs with S-rich surface (S-Ag₂S) are prepared. Ag-Ag₂S and S-Ag₂S show disparate surface configurations: Ag-Ag₂S exposes Ag atoms that bind with NO₃⁻ and octylamine, whereas S-Ag₂S exposes S atoms that bind with two octylammonium ions; both arrangements preserve the charge neutrality. Their ligand exchange reactions by an ion-pair ligand cetyltrimethylammonium bromide (CTAB) are investigated. Two discrete and sequential reactions were observed for Ag-Ag₂S. First, a Br⁻ replaces the initial NO₃⁻ and octylamine ligands (*i.e.*, an X-type and an L-type ligand replaced by one X-type ligand), which concurrently results in coalescence of NCs. The second stage shows strong CTAB adsorption to NC as a whole ion-pair; this process is accompanied by digestive ripening that yields NCs of narrow size distribution. S-Ag₂S show one-to-one positive Z-type to positive Z-type ligand exchange between alkylammonium ions. Ag-Ag₂S has a Lewis acidity/basicity mismatch between the soft surface Ag atom and the hard NO₃⁻ and octylamine ligands, which are replaced by acidity/basicity-matching soft Br⁻. Perchlorate and fluoride fail to achieve this exchange reaction because they are as hard as NO₃⁻. Conversely, CdS NCs which have hard cadmium cations also fail to initiate such ligand exchange by Br⁻. In contrast, S-Ag₂S show unique Z-type to Z-type ligand exchanges that replace octylammonium ion with CTA⁺ or K⁺. This demonstrates how NC surface stoichiometry and surface atom acidity/basicity govern the reactions with ion-pair ligands and subsequent change in NC size and shape.

Symposium : **MAT3-4**

Recent Trends in Infrared Nanomaterials

Room 405 (Live Streaming) THU 16:35

Chair: Kwang Seob Jeong (Korea University)

Design and Application of 0D/2D Hybrid Nanomaterials for Functional NIR Photodetectors

Jong-Soo Lee

Department of Energy Science & Engineering, DGIST, Korea

Colloidal quantum dots and two-dimensional nanomaterials provide a powerful building blocks to engineer optoelectronics devices, opening up new opportunities in the near infrared spectral regions. In this talk, I will introduce recent results regarding hybrid nanomaterials and colloidal quantum dot-based photodetectors toward mid- and long-wavelength infrared. First, I will discuss the synthesis and characterization of various infrared colloidal quantum dots, two-dimensional nanomaterials and hybrid nanomaterials including the basic theory of device operation, the fabrication and measurement of photodetectors, and conclude with the future prospect of this emerging technology.

Second, I will introduce the hybrid photo-FETs combined with the novel properties of the two-dimensional and zero-dimensional nanomaterials as the channel and sensitizer layers. By combining a strong absorbance of a quantum dot (QD) layer and a two-dimensional layer material with high carrier mobility, the hybrid photo-FETs are expected to produce high-performance photodetectors that can effectively control the responsivity, detectivity, and response time.

Symposium : ELEC1-1

New Horizons for Molecular Electrochemistry and Its Applications

Room 406 (Live Streaming) THU 13:10

Chair: Hye Ryung Byon (KAIST)

Electrochemical Monitoring and Mechanistic Understanding of Iodine Film Formation as a Metastable Intermediate during I_3^-/I^- Redox Reaction in Aqueous ZnI_2 Media

Jinho Chang

Department of Chemistry, Hanyang University, Korea

Zn-polyiodide redox flow batteries (RFBs) are a promising grid-scale electrical energy storage (EES) option because of their significant energy density, which is due to the high solubility of ZnI_2 in water. In spite of the importance of the RFBs, a mechanistic understanding of both Zn^{2+}/Zn and I_3^-/I^- half redox reactions have not been fully achieved yet. The I_3^-/I^- half redox reaction occurring on a cathode in this RFB is particularly complicated due to metastable iodine films, which only form on an electrode when an electrochemical potential is biased enough to drive the electro-oxidation of I^- . Due to the thermodynamically unstable nature of iodine films in I^- -rich aqueous solutions, the film is also difficult to characterize by ex-situ analyses, and its physicochemical properties are largely unknown. In this article, we report electrochemical in situ monitoring of the formation and dissolution of a metastable iodine film as an intermediate during I_3^-/I^- redox reactions in an aqueous solution using a rotating ring disk electrode (RRDE). We suggested a reaction model for electro-oxidation of I^- to I_3^- via iodine films and its electro-reduction to I^- based on the mechanism proposed by Gileadi et al. Chronoamperograms (CAs) and cyclic voltammograms (CVs) associated with the I_2/I^- redox reaction involving only formation and dissolution of iodine films on a disk electrode were obtained using an RRDE. From the CAs and CVs, we successfully obtained trajectory information on the formation and dissolution of an iodine film during the I_3^-/I^- redox reaction on a disk electrode under transient and potential-time variation conditions. In addition, we found evidence of a possible transition in the iodine film from an I^- -conductor to an I^- -semiconductor during formation based on the quantitatively monitored iodine formation curve as a function of time during electro-oxidation of I^- .

Symposium : **ELEC1-2**

New Horizons for Molecular Electrochemistry and Its Applications

Room 406 (Live Streaming) THU 13:35

Chair: Hye Ryung Byon (KAIST)

Designing Organic Electrode Materials for Ultra-stable and Fast Rechargeable Batteries

Ji Eon Kwon^{*}, Soo young Park^{1,*}

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

¹Division of Material Engineering, Seoul National University, Korea

With the rapidly increasing demand for batteries as a reliable power source in many different emerging applications, organic electrode materials are drawing much attention as a promising alternative with sustainability and bio-compatibility. Since the first report in 1969, many organic materials showing redox-activity have been studied as electrode materials for various metal-ion batteries. However, their electrochemical performance is still impractical due to intermediate redox potential, high solubility in the electrolyte, and low electric conductivity. In this talk, we present novel p-type redox centers for high-voltage cathode materials with high rate capability. It is revealed that negligible structural reorganization of the redox centers facilitates a kinetically faster electrochemical pathway, leading to a narrow voltage plateau and superior rate capability of the new cathode materials. Finally, we also discuss our more recent results to further improve their cycle stability and specific capacity.

Symposium : **ELEC1-3**

New Horizons for Molecular Electrochemistry and Its Applications

Room 406 (Live Streaming) THU 14:10

Chair: Hye Ryung Byon (KAIST)

Understanding electrochemical CO₂ reduction reaction on the nanoparticle catalyst

Yun Jeong Hwang

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

Electrochemical CO₂ reduction to value-added chemicals has been highlighted as a sustainable carbon cycle technology. Recent material engineering strategies coupled with device designs have made noticeable progress to achieve high conversion rate. Especially, defective structures of the nanoparticle catalysts have shown high intrinsic activity for CO₂RR over hydrogen evolution reaction (HER), and thus high product selectivity. Although nanostructures are advantageous to have high activity and high surface area, the role of the fundamental descriptor allowing control of the desired pathway is not yet well-understood. In this context, reliable guidelines for highly selective reactions and stability require understanding the catalyst material and the reaction pathways. Both of a H-cell and gas-diffusion-electrode (GDE) based membrane electrode assembly (MEA) cells have shown the enhanced CO₂RR with nanoparticles catalysts. In this talk, the recent studies on nanoparticle catalysts will be discussed from the point of fundamental mechanism and durability understanding to the MEA device applications.

Symposium : ELEC1-4

New Horizons for Molecular Electrochemistry and Its Applications

Room 406 (Live Streaming) THU 14:35

Chair: Hye Ryung Byon (KAIST)

Electrochemical biosensors using a photoredox catalyst and a nanozyme

Haesik Yang

Department of Chemistry, Pusan National University, Korea

Two electrochemical biosensors using new catalytic reactions will be presented. In the first part, washing-free DNA detection using surface-plasmonic-field-induced photoredox catalysis will be introduced. A distance-dependent surface plasmonic field induces rapid photoredox catalysis of surface-bound catalytic labels, and distance-dependent mediated electron transfer allows for rapid electron transfer from the surface-bound labels to the electrode. An optimal system consists of a chemically reversible acceptor ($\text{Ru}(\text{NH}_3)_6^{3+}$), a chemically reversible photoredox catalyst (eosin Y), and a chemically irreversible donor (triethanolamine). In the second part, a sensitive immunosensor using a metal nanozyme with ester hydrolysis activity will be introduced. Metal nanoparticle surfaces are used for peroxidase- and oxidase-like nanozymes but not for esterase-like nanozymes. It is found that metal nanoparticle surfaces rapidly catalyze non-redox ester hydrolysis in the presence of redox $\text{H}_3\text{N}-\text{BH}_3$ (AB). Metal hydrides are readily generated on a Pt nanoparticle (PtNP) from AB, and as a result the PtNP becomes electron-rich, which might assist nucleophilic attack of H_2O on the carbonyl group of an ester. The nanozyme system based on PtNP, AB, and 4-aminonaphthalene-1-yl acetate provides an electrochemical signal-to-background ratio much higher than natural enzymes, due to the rapid ester hydrolysis and redox cycling involving the hydrolysis product.

Symposium : ELEC2-1

New Horizons in Physical and Analytical Electrochemistry

Room 406 (Live Streaming) THU 15:10

Chair: Je Hyun Bae (Chungnam National University)

Ion Transport-Coupled Electrochemistry in Confined Nanopore Arrays

Seung-Ryong Kwon, Paul Bohn^{1,*}

Department of Chemistry, Gyeongsang National University, Korea

¹*Department of Chemical & Biomolecular Engineering, University of Notre Dame, United States*

Understanding ion/molecular transport in confined volume is important in designing efficient biomimetic ion channels as well as applications ranging from water separation/purification to molecular-based iontronic devices. Dual electrode-embedded nanopore arrays in metal-insulator-metal configuration are fabricated with a 100 nm distance between electrodes to investigate ion transport in confined geometries. The nanopore electrode arrays enable rapid, repetitive oxidation and reduction of the confined redox species, i.e., redox cycling, inside the nanopores by setting the two electrodes to opposite potentials, leading to a significant faradaic current amplification. Individually encapsulated attoliter-volume nanopores, generated by sealing with a layer of poly(dimethylsiloxane), yield accelerating current enhancement with increasing voltametric scan numbers (or time) up to 250-fold compared to open nanopores. Finite-element simulations reveal that this unprecedented current enhancement originates from two factors: 1) efficient trapping of the redox species in the nanopores; and, more dominantly, 2) enhanced mass transport effects due to solution evaporation. The additional current enhancement beyond simple redox cycling phenomenon owing to the enhanced mass transport effects could be useful for applications such as ultrasensitive sensors and biomimetic solid-state ion channels.

Symposium : ELEC2-2

New Horizons in Physical and Analytical Electrochemistry

Room 406 (Live Streaming) THU 15:35

Chair: Je Hyun Bae (Chungnam National University)

Iontronics

Taek dong Chung

Department of Chemistry, Seoul National University, Korea

Iontronics is an ion-based information processing platform. This was inspired by the neural system, where neurons and synapses act as primary components in signal transmission based on non-linear, dynamic behaviors. Despite the relatively slow operation of individual neurons, their complex network allows high-level information processing such as pattern recognition in human brain, which is infeasible in electronics. In this regard, iontronics can be a prospective candidate that could bridge the gap between solid state electronics and biological system, or even realize neural functions and non-linear characteristics (e.g. plasticity, memory) by employing the same signal carriers and similar operating environments to the neurological system. In this talk, we introduce some of our recent developments in iontronics. Sophisticated designs of microchip-based ionic circuits allowed us to demonstrate ionic diode, transistor, and logic circuits. A fully aqueous ionic circuitry can also be realized by utilizing reverse electro dialysis (RED) as power source. Further, we presented a new methodology to fabricate those iontronic circuits on biocompatible, flexible polydimethylsiloxane (PDMS) microchip, onto which we integrated a mechanical switch and an ionic regulator circuit. Simply by combining ionic circuitry with material properties of PDMS, the ionic regulator exhibits signal transmission characteristics similar to excitatory and inhibitory synapses in the nervous system. Most recently, we demonstrated a polyelectrolyte gel-filled (PGF) micropipette as a chemical delivery probe based on the ion current rectification, which successfully stimulated primary cultured neurons. These examples indicate that iontronics is a promising platform for communication with biological systems.

Symposium : **ELEC2-3**

New Horizons in Physical and Analytical Electrochemistry

Room 406 (Live Streaming) THU 16:10

Chair: Je Hyun Bae (Chungnam National University)

Electrochemical Sensors with Improved Performances via Controlling the Nanostructures of Electrode Materials

Youngmi Lee

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

Electrochemical sensors have attracted great attention continuously due to their unique advantages of simplicity, economical instrumentation, capability of direct and fast analysis with high sensitivity. The analytical performances of electrochemical sensors are known to be varied depending on the properties of electrode materials such as composition and microstructure. In this presentation, a strategy for improving the performances of amperometric sensors via either controlling electrode microstructures or alloying of two immiscible metals. First, electrodeposited platinum (Pt) layers with different nanostructures are characterized for amperometric sensing of nitric oxide (NO). The sensitivity and selectivity to NO are investigated depending on the deposited structures. Second, alloyed nanofibers of highly immiscible gold (Au) and iridium (Ir) are synthesized and applied for direct amperometric sensing of glucose. The sensing performances of sensitivity and selectivity are compared between the composite and alloy of Au and Ir.

Symposium : ELEC2-4

New Horizons in Physical and Analytical Electrochemistry

Room 406 (Live Streaming) THU 16:35

Chair: Je Hyun Bae (Chungnam National University)

Application of modified electrodes for electrochemical biosensors

Yoon Bo Shim^{*}, Kyeong-Deok Seo¹

Department of Chemistry and Institute of Biophysio Sensor technology, Pusan National University, Korea

¹Department of Chemistry, Pusan National University, Korea

In the recent years, numerous biosensors have been studied for medical and health care purposes due to small size and portability, cost effective, simple, and easy operational mode compared to costly and bulky conventional instruments. In this presentation, I want to introduce the strategy for the design and fabrication of modified electrode surface with various catalytic materials for electrochemical biosensor. At first, I will briefly talk about preparation of electrocatalytic mediators for the facile electron transfer and their application to the selective detection of a target species. We synthesized various novel and transition metal nanoparticles having catalytic property towards some selected redox reactions. We also prepared composite electrode materials using conducting polymer to give stable synergistic performance of organic, inorganic, and biological nanomaterials for biosensors. In this regard, metal alloy catalysts for glucose detection and bi-functionalized conducting polymer/N, S-doped carbon for lactate biosensor is worthy to mention. Secondly, I would like to introduce the principal and application of a microfluidic hybrid sensor, where nanomaterials and biological macromolecules can be separated based on the electrohydrodynamic force derived movement. The specialty of this disposable microfluidic device has been made of screen-printed carbon channel on various substrate like glass, polyester film etc. The hybrid sensor has been successfully applied for the separation detection of target species in the complex biomedical samples, such as blood and urine.

Symposium : **ENVR-1**

Advances in Environmental Energy Technologies using sulfur induced materials and reactions

Room 302 (Live Streaming) THU 10:40

Chair: Sungjun Bae (Konkuk University)

Investigating the mechanisms for persulfate activation that depend on the activation strategy and operational conditions

Jaesang Lee

School of Civil, Environmental, Korea

Persulfate activation collectively represents the physicochemical strategies to improve the overall oxidizing capacity of persulfate in two manners i.e., radical and non-radical reaction routes. Similar to the way of converting H₂O₂ into hydroxyl radicals in the conventional advanced oxidation processes, radical-based persulfate activation generates sulfate radicals through the dissociation of peroxide bond in persulfate that occurs via energy or electron transfer. In the non-radical persulfate activation, persulfate as a two-electron oxidant oxidizes nucleophilic anions such as halides and transition metals into highly reactive intermediates, self-decomposes to yield singlet oxygen, and abstracts electrons from organics indirectly relying on the electron-transfer mediating potentials of select metallic and carbonaceous materials. In this presentation, the specific instances of persulfate activation mechanisms described above are introduced along with multiple supporting evidences. The technical merits of select homogeneous and heterogeneous activation processes are also explored based on the comparative assessment in terms of treatment performance and kinetic variation with respect to operation parameters.

Symposium : **ENVR-2**

Advances in Environmental Energy Technologies using sulfur induced materials and reactions

Room 302 (Live Streaming) THU 11:00

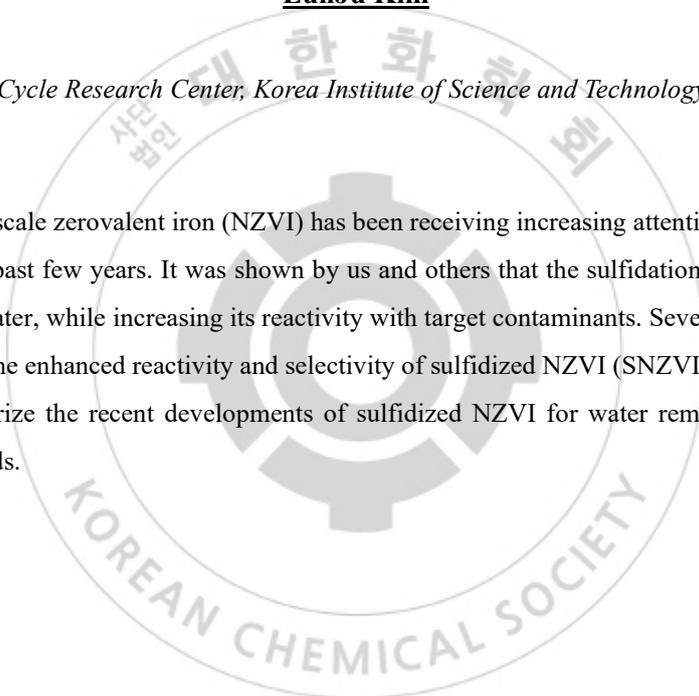
Chair: Sungjun Bae (Konkuk University)

Current understanding of the beneficial effects on sulfidation of iron-based materials for water remediation

EunJu Kim

Water Cycle Research Center, Korea Institute of Science and Technology, Korea

Sulfidation of nanoscale zerovalent iron (NZVI) has been receiving increasing attention for environmental remediation in the past few years. It was shown by us and others that the sulfidation of NZVI suppresses the reaction with water, while increasing its reactivity with target contaminants. Several mechanisms have been proposed for the enhanced reactivity and selectivity of sulfidized NZVI (SNZVI) compared to NZVI. Herein, we summarize the recent developments of sulfidized NZVI for water remediation and suggest future research needs.



Symposium : **ENVR-3**

Advances in Environmental Energy Technologies using sulfur induced materials and reactions

Room 302 (Live Streaming) THU 11:20

Chair: Sungjun Bae (Konkuk University)

Reductive dechlorination of tetrachloroethene enhanced by sulfide-cobalamin in nFeS suspension

Daeseung Kyung

Civil & Environmental Engineering, University of Ulsan, Korea

In this study, we investigated the reductive substitution of aquo-cobalamin(III) (Cbl(III)-H₂O) by sulfide-cobalamin(III) (Cbl(III)-S₂⁻) in the presence of S₂⁻. Cbl(III)-H₂O was transformed to Cbl(III)-S₂⁻ via ligand substitution of H₂O by S₂⁻ at its axial position, due to the weakness of the bond strength of cobalt with H₂O. Cbl(III)-S₂⁻ was reduced to sulfide-cobalamin(II), and partially further to sulfide-cobalamin(I) as the concentration of S₂⁻ increased from 0.1 to 5.0 mM. In the presence of nano-mackinawite (nFeS), Cbl(III)-S₂⁻ species were fully adsorbed onto the nFeS surface and its reactivity was enhanced by the reactive surface chemical species. The dechlorination kinetic rate constant of tetrachloroethene by Cbl(III)-S₂⁻ in nFeS suspension ($k_{\text{nFeS-Cbl(III)-S}_2^-} = 0.008 \pm 0.001 \text{ hr}^{-1}$) was 4 times greater than that by Cbl(III)-H₂O, showing a potential role for $\equiv\text{S}_2^-$ -Cbl(II) as a more effective electron transfer mediator than $\equiv\text{S}_2^-$ -Cbl(II) and $\equiv\text{OH-Cbl(II)}$. The experimental results provide fundamental knowledge on potential biogeochemical reactions relevant to interactions between S₂⁻ and bacterial coenzyme in nFeS suspension, which can significantly enhance reductive dechlorination of chlorinated compounds in contaminated sites.

Symposium : **ENVR-4**

Advances in Environmental Energy Technologies using sulfur induced materials and reactions

Room 302 (Live Streaming) THU 11:40

Chair: Sungjun Bae (Konkuk University)

Remediation of heavy metal contaminated acidic groundwater using sulfidated zerovalent iron: batch and column tests

Yu-Gyeong Kang, In-Gyu Song, Yoon-seok Chang^{1,*}

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

¹*Division of Environmental Engineering, Pohang University of Science and Technology, Korea*

High concentrations of cadmium, zinc, and aluminum have been detected in the groundwater near Yeongpoong Seokpo Refinery, causing serious environmental and social problems. A recent study found that sulfidated nanoscale zerovalent iron (S-nZVI) can provide high reactivity with cadmium by replacing Fe of FeS with Cd. In this study, S-nZVI and S-nZVI based all-in-one mixture were applied to remediate groundwater from Yeongpoong Seokpo Refinery in batch and column tests. The groundwater was extremely acidic with pH 2.7 and the initial concentrations of heavy metal were 81.2 mg/L (Cd), 988.7 mg/L (Zn), 119.8 mg/L (Al), and 3.7 mg/L (Cu), respectively. As a result, acryl column (length 18 cm, diameter 4 cm) filled with sand and 10 g of S-nZVI maintained removal efficiency of heavy metals (Cd, Zn, Al, and Cu) higher than 90% for 10 hours, but gradually decreased during 232 hours of reaction. The pH increased higher than 4 and ORP decreased from 400 mV to 230~270 mV as the S-ZVI reacted with oxygen and water. However, the leaching of Fe ions was significant with a peak concentration of 1200 mg/L. To overcome this limitation, we developed an all-in-one mixture of S-nZVI, CaCO₃, and activated carbon by simply mixing the constituents. The mixture dramatically decreased the concentration of iron ion and increased the pH higher than 6 in batch tests. The column tests of the mixture will be conducted after optimization of the constituent ratio. Lastly, the reaction mechanism of S-nZVI and mixture will be elucidated by analyzing the particles after the reaction using SEM, EDX, FT-IR, XRD, and XPS.

Symposium : **EDU-1**

Current Trends in Chemistry Education

Room 302 (Live Streaming) THU 15:00

Chair: Hyun Jung Kim (Kongju National University)

Issues on Forth-coming National Curriculum Reform Emphasizing Students' Choice

Dae Hong Jeong

Department of Chemical Education, Seoul National University, Korea

Korean government prepares National Curriculum Reform in 2022, which is in 7 years since the previous National Curriculum Reform in 2015. This reform emphasizes on widening students' choice of subjects in high school considering students' various interests and future carriers. Although this goal itself is reasonable, many people worry on the side effect of this approach considering high competition of entrance to high-rank universities and under-registration of low-rank universities. One of typical example is that students can choose "Chemistry I" and any one subject in "Society Subject" for high rank score of University Entrance Examination. Then, they don't study "Chemistry II" even if they proceed to chemistry-related department in universities. In this talk I would like to reveal several issues raised by many stake-holders in chemistry education in high school. I can show a few suggestion on the forth-coming curriculum reform and have chance to listen to the chemistry society.

Symposium : **EDU-2**

Current Trends in Chemistry Education

Room 302 (Live Streaming) THU 15:30

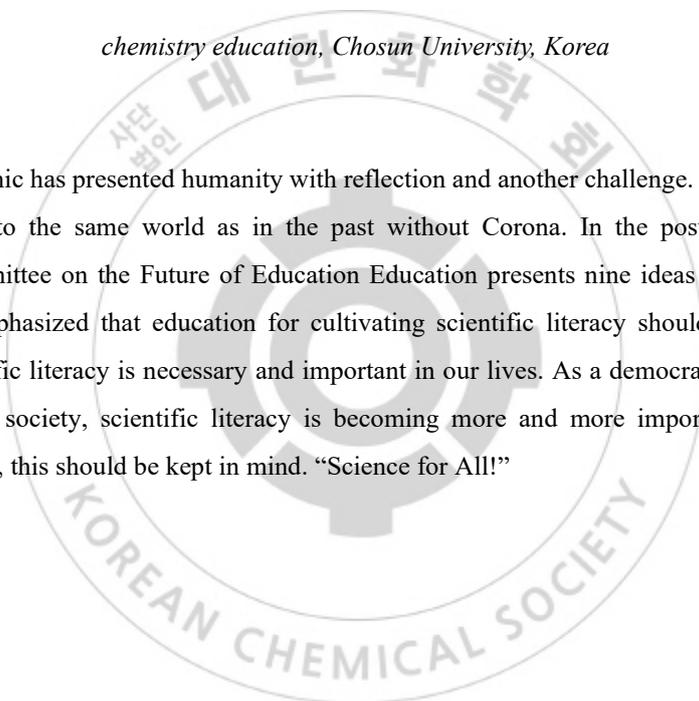
Chair: Hyun Jung Kim (Kongju National University)

Revising National Chemistry Curriculum for K-12

HyunJu Park

chemistry education, Chosun University, Korea

The COVID epidemic has presented humanity with reflection and another challenge. Everyone knows that we can't go back to the same world as in the past without Corona. In the post-COVID world, the International Committee on the Future of Education Education presents nine ideas for public action. In particular, it is emphasized that education for cultivating scientific literacy should be included in the curriculum. Scientific literacy is necessary and important in our lives. As a democratic citizen in modern science-technology society, scientific literacy is becoming more and more important. In revising the national curriculum, this should be kept in mind. "Science for All!"



Symposium : EDU-3

Current Trends in Chemistry Education

Room 302 (Live Streaming) THU 16:00

Chair: Hyun Jung Kim (Kongju National University)

Comparative Analysis of Chemistry Curriculum between Korea and Estonia

Hyun Jung Kim

Chemistry Education, Kongju National University, Korea

The 2022 curriculum revision and the 2025 high school credit system are coming soon. Students choose the subjects they need to take through selection, and the school must be able to organize subjects to meet various needs. To this end, it is thought that it is necessary to open courses that meet the number of units and social needs. Therefore, we will look at the chemistry curriculum in Estonia, which is evaluated as an emerging education power in Europe and an IT powerhouse leading the 4th industrial revolution, and compare it with the chemistry curriculum in Korea. Since both countries are operating national curriculum, we intend to analyze based on curriculum documents. Mainly, it is intended to compare the composition of chemistry subjects within the science curriculum, science subject competencies, content elements by grade, ICT use in class, achievement standards, and evaluation. In addition, we will look at creative work, which is a requirement for graduation, and project classes using robots. Based on this, we are going to look at the implications of revising the curriculum in the future.

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

Oral Presentation for Young Polymer Scientists

Room 403 (Live Streaming) THU 09:00

Chair: Jeewoo Lim (Kyung Hee University)

Well-defined Semifluorinated Norbornene Polymerization through Fluorous Block Copolymer Surfactants

Sanghoon Song, Jeewoo Lim*

Department of Chemistry, Kyung Hee University, Korea

High fluorine-content polymers have a variety of unique chemical and physical properties, and this has led to the development of numerous synthetic approaches toward well-defined fluoropolymers. Most synthetic methods reported to date have limitations which include the use of expensive fluorinated solvents, low molecular weight ($M_n < 3.5$ kDa) products, and confined monomer scope (acrylates and methacrylates). Herein, we report the synthesis of highly fluorinated block copolymers using living ring-opening metathesis polymerization (ROMP). These block copolymers are performed as excellent surfactants that stabilize the homopolymerization of a highly fluorinated monomer having fluorine content of over 60 wt%. The use of fluorinated surfactants allowed for the polymerization of the highly fluorinated monomer in general organic solvents, such as dichloromethane or tetrahydrofuran. Notably, the use of the block copolymer surfactant increased the rate of homopolymerization by more than 1,000-fold, and gave fluoropolymers with very high molecular weights (of over 200 kDa) and narrow molecular weight distributions ($\mathcal{D} < 1.2$). The resulting fluoropolymers were obtained as polymer nanoparticles, the size of which could be controlled by varying the polymerization parameters.

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

Oral Presentation for Young Polymer Scientists

Room 403 (Live Streaming) THU 09:12

Chair: Jeewoo Lim (Kyung Hee University)

Impact of Molecular Weight on Molecular Doping Efficiency of Conjugated Polymers and Resulting Thermoelectric Performances

Bomi Kim, BongSoo Kim*

Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Korea

We studied that the effect of molecular weight of a series of CPs based on DFD moiety on the doping efficiency, electrical conductivity, and related thermoelectric properties of doped-CPs. Low, medium, and high batches of PDFD-T polymers were synthesized and labeled as PDFD-T(L), PDFD-T(M), and PDFD-T(H), respectively. To compare the effect of different donor moieties, donor units of PDFD-T(L) were also structurally modified to PDFD-TT(L) and PDFD-DTT(L). After doping those CPs with FeCl₃, d-PDFD-T(H) exhibited electrical conductivity over 400 S/cm, which is significantly higher than d-PDFD-T(L), d-PDFD-T(M), d-PDFD-TT(L), and d-PDFD-DTT(L). According to the results of various characterizations including UV-Vis-NIR spectroscopy, charge carrier mobility, electrical conductivity, Hall effect and GIWAXS measurements, we demonstrated that the molecular weight of CPs is directly related to the crystallinity of the CP films, which affects resulting charge carrier mobility. The lower molecular weight CPs, the lower carrier mobility was shown in spite of the same chemical structures. It is because crystalline grains were deteriorated critically after doping, while high molecular weight CPs maintained its original morphology and high carrier mobility. Even for the CPs with stronger electron donating units, low molecular weight adversely affected morphological and electrical features. In conclusion, using PDFD-T(H), we achieved the highest power factor over 100 $\mu\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-2}$, which is among the highest levels for doped CPs. Our work suggests that the controlling molecular weight of CPs can provide a key solution to minimize the crystallinity degradation of doped-CPs, ultimately to optimize the doping efficiency, electrical conductivity, and thermoelectric properties.

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

Oral Presentation for Young Polymer Scientists

Room 403 (Live Streaming) THU 09:24

Chair: Jeewoo Lim (Kyung Hee University)

Solvent effect in photoinduced electron/energy transfer-reversible addition-fragmentation chain transfer (PET-RAFT) polymerization for vinyl acetate

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*

Photoinduced electron/energy transfer reversible addition-fragmentation chain transfer (PET-RAFT) polymerization, one of the controlled radical polymerizations (CRP), is catalyzed photocatalysts which absorb the light and become a photoexcited state. Over the past decade, PET-RAFT polymerization has attracted interest for the production of the well-defined polymer and narrow the molecular weight distribution allowing temporal and spatial control of the light source. Although most of the PET-RAFT polymerizations are reacted in a diluted system, however, the solvent effect is not deeply studied. Herein, we explored solvent effect in PET-RAFT polymerization of vinyl acetate in the presence of xanthate derivative as a chain transfer agent. It was observed that the monomer conversion and degrees of control were deviated along with solvent polarity. Combined with quantum calculations (TD-DFT), the solvent effect was investigated and poly(vinyl acetate) was synthesized under the visible light.

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

Oral Presentation for Young Polymer Scientists

Room 403 (Live Streaming) THU 09:36

Chair: Jeewoo Lim (Kyung Hee University)

Chemical Upcycling of Waster Ploy(bisphenol A carbonate) to 1,4,2-dioxazolones

Hyun Jin Jung, Jeung Gon Kim*

Department of Chemistry, Jeonbuk National University, Korea

Poly(bisphenol A carbonate) (PC) is a leading engineering plastic having high heat and impact resistance and transparency. Annually, over 5 million tons PC is consumed. However, the attention of its recycling has not been given despite environmental concerns of bisphenol A. Most of waste PC goes to landfill, its chemical degradation and monomer recovery have been studied, called chemical recycling. While the recovery of bisphenol A was a primary goal, the leftover carbonyl moiety still can be a valuable in carbonylation reactions. We have developed an efficient synthetic protocol of 1,4,2-dioxazolones beginning from hydroxamic acid and PC. With a proper organic catalyst, the waste PC was degraded into bisphenol A and the corresponding 1,4,2-dioxazolones, quantitatively. The details of condition optimization, scope, and utilization will be disclosed.

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

Oral Presentation for Young Polymer Scientists

Room 403 (Live Streaming) THU 10:00

Chair: Jeewoo Lim (Kyung Hee University)

Structure and Dynamics of Antifreeze Hydrogels Based on Multiple Hydrogen Bonding

Jewon Choi, Kookheon Char*

Chemical & Biological Engineering, Seoul National University, Korea

Hydrogels based on dynamic physical junctions have recently attracted immense interest since the reversible bonds can endow functional properties such as self-healing and injectability. Particularly, ureidopyrimidinone groups (UPy) composed of quadruple hydrogen bonds have been used as the reversible crosslinkers for physically-bonded hydrogels or elastomers. In the present study, random copolymer hydrogels containing a large amount of UPy (35 ~ 45 wt%) were synthesized and mechanical, structural, and antifreeze properties of such hydrogels were characterized. The hydrogels are self-healable and also exhibit injectable properties due to their reversible nature of the physical bonds. In addition, the small-angle X-ray scattering reveals the presense of water-impermeable domains in the hydrogel and the nano-confinement of water molecules between them. The confined water molecules are hardly frozen during the freezing process or, at least, they become metastable even if they are crystallized. In addition, the frequency-dependent rheology reveals that the dynamics of UPy becomes slow at low temperature, leading to the confinement formation based on the stacking of UPy dimers. Controlled dynamics of the UPy domains induces both antifreeze and self-healable properties and we hope that this finding would aid in designing of water-soluble functional hydrogels for diverse applications.

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

Oral Presentation for Young Polymer Scientists

Room 403 (Live Streaming) THU 10:12

Chair: Jeewoo Lim (Kyung Hee University)

Decision of supramolecular chirality in interplay between photonic and molecular chiralities

Jun Su Kang, Woo youn Kim¹, Myungeun Seo^{*}

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

¹*Department of Chemistry, KAIST, Korea*

A small amount of primal chiral bias caused by circularly polarized light (CPL) is tenably considered one of the key sources to homochirality in nature that is amplified from a molecular scale to mesoscopic and macroscopic levels. Here we report development of supramolecular chirality via co-assembly of chiral and achiral triphenylamine derivatives upon irradiation of both directions of CPL. We trace growth supramolecular helices by temperature-dependent experiments and simulations. Possibilities of amplifying and overriding molecular chirality by CPL will be discussed to shed light on evolution of homochirality.

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

Oral Presentation for Young Polymer Scientists

Room 403 (Live Streaming) THU 10:24

Chair: Jeewoo Lim (Kyung Hee University)

Degradable Sugar-Based Polymers via Cascade Metathesis Polymerization

Gregory Peterson, Tae-Lim Choi^{1,*}

Chemistry, Incheon National University, Korea

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

Enyne monomers derived from xylose underwent cascade metathesis polymerizations to prepare new polymers with a ring-opened sugar and degradable linkage incorporated into every repeat unit of the backbone. Polymerizations were well-controlled and had living character, which enabled the preparation of high molecular weight polymers with narrow molecular weight dispersity and block copolymers. By tuning the type of acid-sensitive linkage, we could change the degradation profile of the polymer and the identity of the resulting degradation products. For instance, a large difference in degradation rates between hemi-aminal ether and ether-based polymers was observed, enabling the sequential degradation of a block copolymer. Furthermore, we exploited the generation of furan-based degradation products, from an acetal-based polymer, to achieve the release of covalently bound reporter molecules upon degradation.

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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 402 (Live Streaming) THU 09:00

Chair: Seung Jun Hwang (POSTECH)

Recent Electron Microscopy Techniques for Inorganic Materials

Joohyun Lim

Department of Chemistry, Kangwon National University, Korea

Electron microscopy and related analytical methods have been applied to investigate the size, morphology, crystal structure, atomic arrangement, and chemical composition of inorganic materials. The obtained information is used to determine the growth mechanism of nanostructures and structure-properties relationships. The investigated characterizations are beneficial in various applications such as rechargeable batteries, electrocatalysts, solar-cells, etc. However, the full characterization of inorganic materials using conventional electron microscopy techniques is still challenging. Recently, new electron microscopy strategies are being developed to optimize the properties and increase the stability of the functional materials. In this talk, state-of-the-art electron microscopy techniques are introduced for the in-depth characterization of functional inorganic materials. In particular, transmission electron microscopy, electron tomography, electron energy loss spectroscopy, focused ion beam, and atom probe tomography are discussed. Finally, the detailed applications, limitations, and future research direction will be discussed.

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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 402 (Live Streaming) THU 09:15

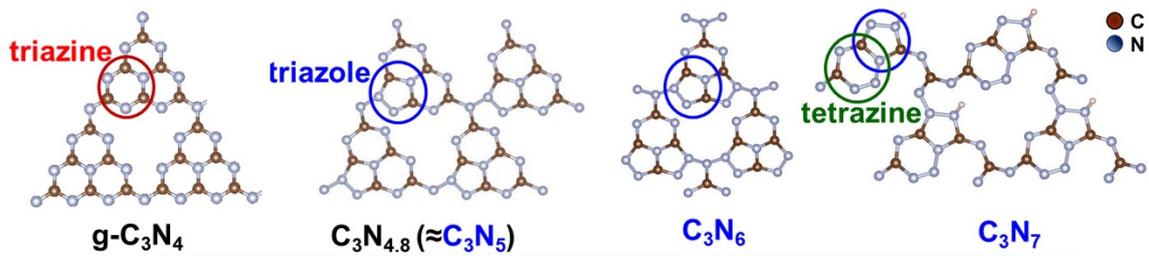
Chair: Seung Jun Hwang (POSTECH)

Triazole-based Carbon Nitrides

In Young Kim

Department of Chemistry, Chonnam National University, Korea

The 5 types of crystal structures of C_3N_4 have been known so far. Among them, graphitic carbon nitride (g- C_3N_4) have attracted significant research interest due to its huge potential as a benign material for production of sustainable energy including hydrogen. The crystal structure of g- C_3N_4 is the layered structure composed of extended heptazine unit. Generally, chemical modification such as introducing heteroatoms and/or altering crystal structure significantly affects physicochemical properties of materials. Although it is expected that nitrogen-enrichment in the g- C_3N_4 would bring merits to improve its functionalities in energy storage and conversion, synthesis of nitrogen-enrich carbon nitride was the biggest hurdle in proving it owing to thermodynamic instability of N-N bond. Recently, we overcame this barrier by adopting 5-amino-1H-tetrazole as a precursor to synthesize nitrogen-rich carbon nitrides during pyrolysis at a relatively low temperature (≤ 400 °C). Interestingly, the 5-amino-1H-tetrazole-derived carbon nitrides with $C_3N_{4.8}$ ($\approx C_3N_5$), C_3N_6 and C_3N_7 compositions show strong evidences being composed of triazole and/or tetrazine units instead of heptazine unit. We for the first time have denoted these nitrogen-enrich carbon nitrides as triazole-based carbon nitrides. In this talk, the crystal structures and physicochemical properties of the triazole-based carbon nitrides will be introduced with a perspective on their applications in the fields of energy storage and conversion. References: 1.S. Kim, M. Hankel, W. Cha, G. Singh, J. M. Lee, I. Y. Kim, A. Vinu, Nano Energy 2020, 72, 104702. 2.I. Y. Kim, S. Kim, S. Premkumar, J. -H. Yang, S. Umaphathy, A. Vinu, Small 2020, 16, 1903572. 3.I. Y. Kim, S. Kim, X. Jin, S. Premkumar, G. Chandra, N. -S. Lee, G. P. Mane, S. -J. Hwang, S. Umaphathy, A. Vinu, Angew. Chem. Int. Ed. 2018, 57, 17135-17140.



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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 402 (Live Streaming) THU 09:30

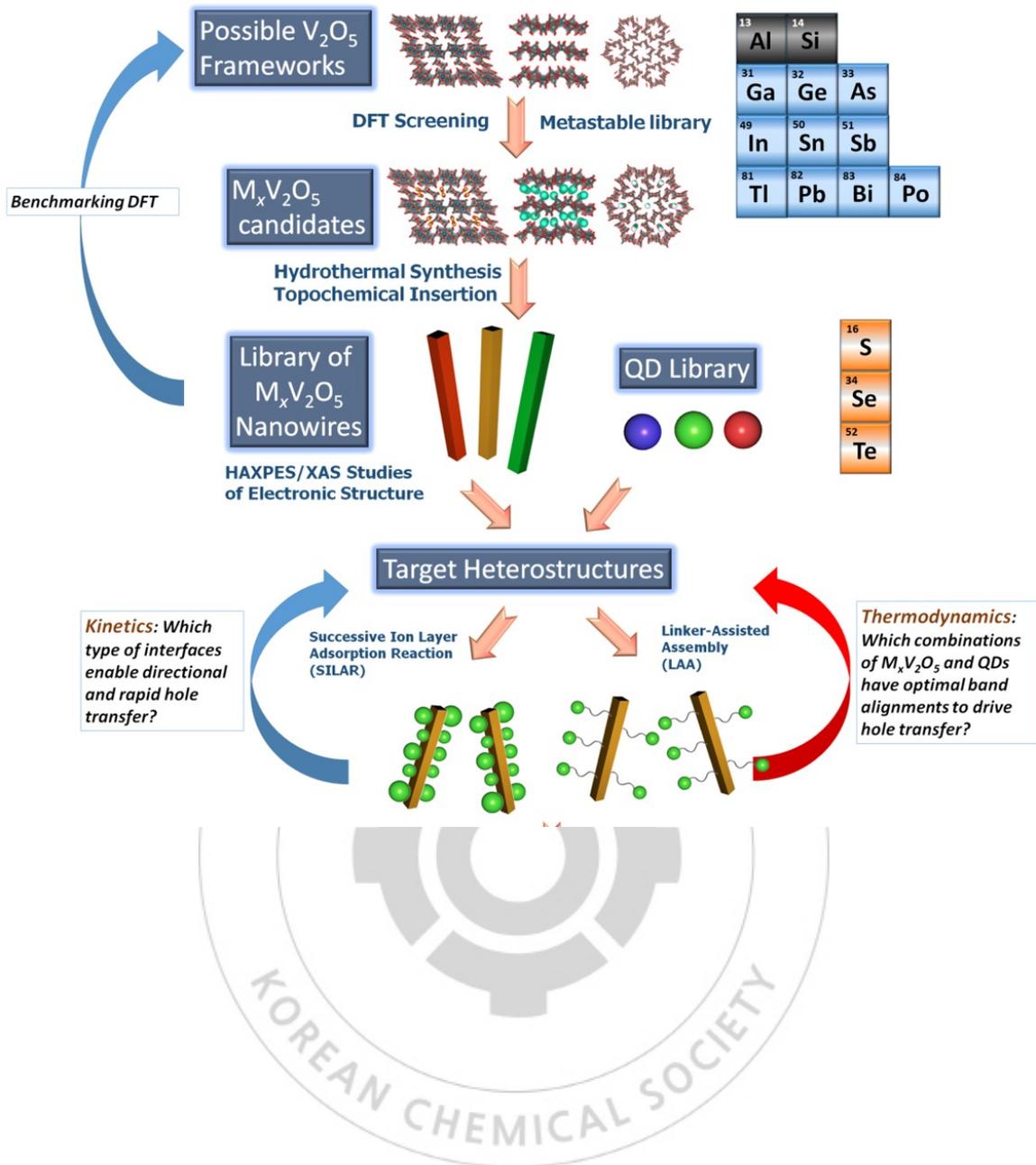
Chair: Seung Jun Hwang (POSTECH)

Rational Design of Inorganic Semiconductor Heteronanostructures for Solar Energy Conversion

Junsang Cho

Department of Chemistry, Duksung Women's University, Korea

Given increasing worldwide energy consumption, the development of efficient solar energy conversion to augment other renewable energy approaches is one of the grand challenges in our time. Water splitting, or the disproportionation of H₂O into energy-dense fuels, H₂ and O₂, is undoubtedly a promising strategy to store energy in chemicals. However, solar water splitting has been a long challenge in the scientific community since the process involves the concerted transfer of four electrons and four protons, which requires the synergistic operation of solar light harvesting, charge separation, mass and charge transport, and redox catalysis processes. Here, we present the development of tunable and programmable heterostructures using low dimensional nanostructure as photocatalytic platforms including two-dimensional (2D) MoS₂ and one-dimensional (1D) MxV₂O₅ nanowires (where M = Pb²⁺, Sn²⁺) and in couple with quantum dots (QDs: CdS, CdSe, and CdTe). Operation of the desired sequence of light harvesting, charge separation, and charge transport events within heterostructures is governed by the thermodynamic energy offsets of the two components and their photoexcited charge-transfer reactivity, which determine the extent to which desirable processes can outcompete unproductive recombination channels, which have been studied by hard X-ray photoelectron spectroscopy and density functional theory, whereas the dynamics of charge transfer kinetics has been examined by ultrafast transient absorption spectroscopy. The accurate mapping of thermodynamic driving forces and dynamics of charge transfer in these heterostructures suggests a means of engineering ultrafast electron transfer and effective charge separation to design viable photocatalytic architectures.



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

Oral Presentation of Young Scholars in Inorganic Chemistry

Room 402 (Live Streaming) THU 09:45

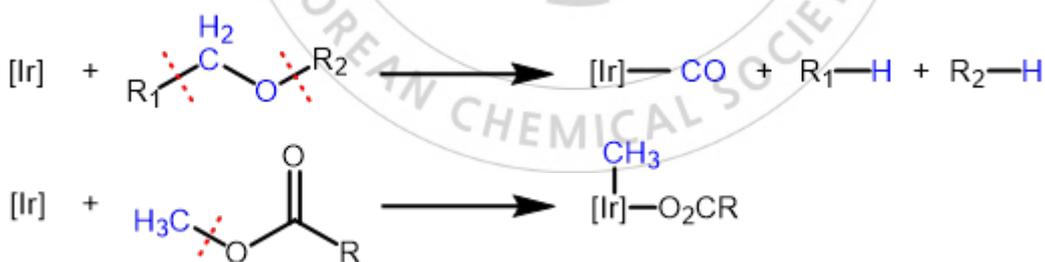
Chair: Seung Jun Hwang (POSTECH)

C-O bond activation by organometallic iridium(I) complexes

Changho Yoo

Department of Chemistry, Korea Research Institute of Chemical Technology, Korea

The activation of C–O bonds offers opportunities in synthesis. In particular, C–O bond activation of ether and ester is receiving great attention due to their prevalence in organic synthesis and biomass conversion. Here, activation of ether and ester C–O bond by organometallic iridium complexes is presented. The intramolecular C–O cleavage of a ligand ether moiety was discovered while attempting to prepare iridium(I) compounds. Mechanistic studies shows initial C–H activation and carbene formation by iridium(I) species to precede productive C–O bond activation. The intermolecular activation of ether and ester was investigated using isolated iridium(I) complexes with an ether-free ligand.



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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 09:00

Chair: Ilsun Yoon (Chungnam National University)

Study on structures of individual conformers by IR depletion/dip VUV-MATI spectroscopy

Sung Man Park, Chan Ho Kwon*

Department of Chemistry, Kangwon National University, Korea

We have measured the high-resolution vibrational spectra of various molecular cations through one-photon vacuum ultraviolet mass-analyzed threshold ionization (VUV-MATI) spectroscopy and conducted the quantum chemical calculations to elucidate the conformations of the neutral and the cationic molecules. In general, conformational studies using one-photon MATI spectroscopy can be explored under various molecular beam conditions. However, in the case that the conformational stability is very small, the quantum chemical calculation results may be inconsistent due to an error in energy calculation. In that regard, we developed the conformer-specific vibrational spectroscopic techniques to obtain the identifiable vibrational spectra of individual conformers in the neutral and the cationic states. In detail, the conformer-selected vibrational spectrum of each neutral conformer could be measured through the IR dip VUV-MATI spectroscopy, whereas the conformer-selected vibrational spectrum of each cationic conformer could be measured by the IR depletion VUV-MATI spectroscopy based on the IR dip VUV-MATI spectra. As a result, we could identify the individual conformers suggested by the one-photon VUV-MATI spectroscopy.

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 09:08

Chair: Ilsun Yoon (Chungnam National University)

Broadband Mid-infrared Dual Frequency Comb Spectroscopy of Condensed Phases

Noh Soo Han, Minhaeng Cho^{1,*}

Center for Molecular Spectroscopy and Dynamics, Institute for Basic Science, Korea

¹*Department of Chemistry, Korea University, Korea*

Mid-infrared (mid-IR) spectroscopy provides a way to study structures and dynamics of complicated molecules in condensed phases. Therefore, developing compact and broadband mid-IR spectrometer has been a long-standing challenge. Recently, as an alternative radiation source for molecular spectroscopy in the mid-IR frequency region, optical frequency comb (OFC) technologies have been used to develop mid-IR frequency combs for high resolution rovibrational spectroscopy of molecules in condensed phases as well as in the gas phase, where the Fourier-transform (FT) spectra were calibrated directly by the frequency-resolved comb-tooth spacing. Dual frequency comb spectroscopy has been found to be exceptionally useful for an interferometric detection of free-induction-decay signal in various linear and nonlinear optical spectroscopic studies. In this presentation, I'll show that a highly coherent and broadband mid-IR frequency comb can be generated by using an intra-pulse difference-frequency-generation with a train of pulses from a few-cycle Ti:Sapphire oscillator. By tightly focusing the oscillator output beam into a single-pass fan-out-type periodically-poled lithium niobate crystal and tilting the orientation of the crystal with respect to incident beam, it is shown that mid-IR frequency comb with more than an octave spectral bandwidth from 1550 cm^{-1} (46 THz) to 3650 cm^{-1} (110 THz) and vanishing carrier-envelope offset phase can be generated. Then, using two coherent mid-IR frequency combs, we demonstrate that ultrabroad mid-IR dual frequency comb spectroscopy of both aromatic compound and amino acid in solutions is experimentally feasible.

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 09:16

Chair: Ilsun Yoon (Chungnam National University)

Photocatalytic activity of commercial rutile TiO₂ mixed cement towards NO oxidation under visible light for air purification.

Soong Yeon Kim, Saqlain Shahid, Shufang Zhao, Young Dok Kim *

Department of Chemistry, Sungkyunkwan University, Korea

To apply photocatalyst in construction field, many researchers have studied to mixing it with binders for several decades. It has been difficult to apply photocatalyst to products in construction field for various reasons such as photocatalytic activity and cost-effectiveness. Nevertheless, studies which are optical, chemical, and physical relationships between photocatalyst and binder have not been conducted. In previous studies, we confirmed the importance of the relationships to mixing two different photocatalysts and binder. In this study, two different rutile TiO₂ (R996 and P25 annealed at 750°C) were mixed with cement and their photocatalytic activities towards NO oxidation were investigated because the rutile TiO₂ which was P25 annealed at 750°C was visible light-driven. The activity photocatalytic activity of cost-effective R996 in cement showed higher photocatalytic activity and NO₃⁻ selectivity compared to annealed P25. The photocatalytic activities of various contents of R996 or Fe-R996 in cement were also investigated because Fe loading on TiO₂ showed photocatalytic enhancement effect. And the mixtures were analyzed by SEM, XRD, PL, UV-DRS, XPS to check structural properties, optical properties, and chemical oxidation states. The different loading amount of R996 mixed with cement on SUS plate was additionally evaluated to photocatalytic activity. Based on those results, the activity was attributed to the number of interfaces between TiO₂ and cement. Furthermore, the operando DRIFTS was used to further understand reaction mechanism. Therefore, we suggest that the cost-effective R996 is suitable photocatalysts to apply in construction field for air purification.

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 09:24

Chair: Ilsun Yoon (Chungnam National University)

Enhanced removal of toluene over nitric acid modified activated carbon under visible light irradiation

Saqlain Shahid, Soong Yeon Kim, Shufang Zhao, Young Dok Kim *

Department of Chemistry, Sungkyunkwan University, Korea

Commercial activated carbon (AC) was used for the removal of toluene under different relative humid (RH) conditions (0, 30, and 60% RH) with and without visible light irradiation. Under each humid condition enhanced removal of toluene was observed under visible light irradiation compared to the absence of light. And when the commercial AC was treated with nitric acid solution of an optimized concentration its toluene removal efficiency was further enhanced under visible light irradiation at 60% RH. Photoinduced oxidation of toluene upon nitric acid modified AC was confirmed by comparing Fourier transform infrared (FT-IR) spectra before and after toluene removal experiments. Toluene removal efficiency of the spent AC sample was also reversed by using a very cheap regeneration method. Moreover, when mixed with white cement nitric acid modified AC also showed increased toluene removal under visible light irradiation compared to dark condition which depicts its feasibility for various indoor and outdoor air purification applications.

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 09:32

Chair: Ilsun Yoon (Chungnam National University)

Electronic dynamics of self-doped HgS colloidal quantum dots: Ultrafast intraband Auger process

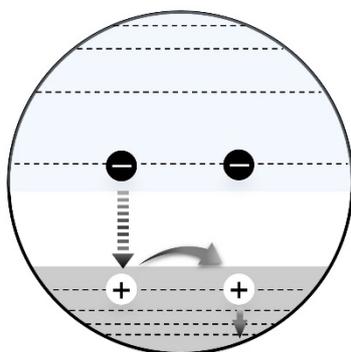
Joonhyung Lim, Minhaeng Cho^{1,*}, Kyungwon Kwak^{1,*}, Kwang Seob Jeong^{1,*}

Center for Molecular Spectroscopy and Dynamics, Korea University, Korea

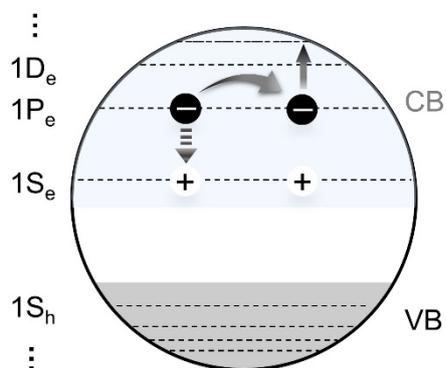
¹Department of Chemistry, Korea University, Korea

The selective study of electronic dynamics in the conduction band (CB) is important for the fundamental understanding of colloidal quantum dots (CQDs) but challenging. To investigate the electronic dynamics of CQDs with empty CB states, the electronic transition from the valence band (VB) to CB (i.e. interband photoexcitation) is necessary. This interband transition inevitably creates a hole in the VB. Due to the different energy gaps between neighboring states in each band and the characteristic effective masses, a hole in the VB and an electron in the CB exhibit different dynamics. To study the electronic dynamics in the CB selectively, n-Type self-doped CQDs were studied with time-resolved mid-infrared spectroscopy. The self-doped CQDs, with excess electrons occupying the low-lying state in the CB, offers a platform for studying electron dynamics without contributions from holes in the VB. We can show an ultrafast intraband Auger process, electron relaxation between spin-orbit coupling states, and exciton-to-ligand vibrational energy transfer process that all occur in the CB of the self-doped HgS CQDs.

Interband Auger process



Intraband Auger process (IAP)



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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 09:40

Chair: Ilsun Yoon (Chungnam National University)

Chemical and geometric control of molecular diffusion and redox in 2D van der Waals space

Haneul Kang, Sunmin Ryu*

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

Understanding molecular behavior in nanometer-scale confinement is important in various scientific fields and technological applications of low-dimensional material systems. Investigation of molecular diffusion in nanometer-sized space has remained largely unexplored because reliable confinement systems and sensitive spectroscopic probes have been lacking. In this work,[1] we show that interfacial diffusion of O₂ molecules and their subsequent reduction through charge transfer (CT) can be controlled by geometric or chemical manipulation of the vdW interface between single layer transition metal dichalcogenides (TMDs) and dielectric substrates. As an indirect but sensitive probe for molecular diffusion, photoluminescence (PL) from TMDs was used in a wide-field imaging mode.[2] Interfacial diffusion of the molecular dopants was accelerated for samples with larger interfacial gaps between TMDs and supporting substrates. We also show that the widely varying CT kinetics of four TMDs originates from their native defects which serve as CT centers. Furthermore, spatiotemporal propagation of CT could be drastically modulated by introducing additional defects on either side of TMDs.[1] H. Kang and S. Ryu,* “Chemical and Geometric Control of Molecular Diffusion and Redox in 2D van der Waals Space”, to be submitted[2] K. Park, H. Kang, S. Koo, D. Lee and S. Ryu,* “Redox-Governed Charge Doping Dictated by Interfacial Diffusion in Two-Dimensional Materials”, Nature Commun. 10, 4931 (2019)

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 09:48

Chair: Ilsun Yoon (Chungnam National University)

Direct Observation of Structural Dynamics Manipulating the Fate of the Excimer State by Ultrafast Time-domain Raman Spectroscopy

Yongseok Hong, Woojae Kim¹, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

¹*Department of Chemistry and Chemical Biology, Cornell University, United States*

In π -conjugated organic photovoltaic devices, an excimer state has been generally regarded as a trap state which hinders efficient excitation energy and charge transport. However, it has been reported that the excimer often acts as an intermediate, which can be further relaxed to the charge-separated or multiexcitonic triplet pair state, suggesting the potential of the excimer state for the manifestation of desirable photophysical properties in photovoltaic devices. Although it has been suggested that the structural dynamics after photon absorption is crucial for the excimer formation in molecular aggregates, direct tracking of the accompanying structural changes has remained unexplored. Here, we present the landscape of structural evolution from the excimer formation to its relaxation in an archetypical perylene bisimide folda-dimer using ultrafast time-domain Raman spectroscopy. First, we directly probed the ultrafast structural evolution triggering 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 reveals that the ring deformation mode, which is tunable through the structural distortion, plays a crucial role in controlling the 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.

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 09:56

Chair: Ilsun Yoon (Chungnam National University)

Davydov Splitting, Superradiance and Evolution of Molecular Excitons in Two-Dimensional PTCDA Crystals

Sunmin Ryu^{*}, Dogyeong Kim

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

Two-dimensional (2D) van der Waals materials have recently gained much research interest because of their potential in various applications. Unlike 2D atomic crystals represented by graphene, MoS₂, and hexagonal BN, however, 2D molecular crystals have rarely been studied. In this work,[1] single and few-layer PTCDA (perylene-3,4,9,10-tetracarboxylic dianhydride) crystals were grown on hexagonal BN by self-limited vapor assembly. Polarized photoluminescence (PL) spectra revealed Frenkel and Charge transfer (CT) excitonic emissions with a strong dependence on thickness. The former exciton exhibited significant vibronic progressions with pronounced Davydov splitting for 0-0 peak, indicating the presence of multiple basis molecules in a unit cell, which was also confirmed in absorption spectra. The temperature-dependence of PL signals suggested thermal equilibration between the two Davydov states and revealed coherence-derived superradiance affecting their spectral width and energy. By determining transition dipole moments using polarized PL analysis, we also directly show the CT character in the Frenkel exciton is enhanced for thicker layers with increased π - π interactions due to Frenkel-CT mixing. Reference[1] D. Kim and S. Ryu,* "Davydov Splitting, Superradiance and Evolution of Molecular Excitons in Two-Dimensional PTCDA Crystals", to be submitted (2021)

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 10:04

Chair: Ilsun Yoon (Chungnam National University)

Surface enhanced Raman spectroscopy reveals the Hydration Water Character on Atomically Dislocated Surfaces

Dongha Shin

department of chemistry, Inha University, Korea

Hydration is ubiquitous in any kind of water–substance interaction such as in various interfacial and biological processes. Despite substantial progress made to date, however, still less explored is the hydration behavior on complex heterogeneous surfaces, such as the water surrounding the protein, which requires a platform that enables systematic investigation at the atomic scale. Here, we realized a heterogeneous self-assembled monolayer system that allows both controllable mixing with hydrophobic or hydrophilic groups and precise distance control of the functional carboxyl groups from the surface by methylene spacer groups. Using surface-enhanced Raman spectroscopy (SERS), we first demonstrated the hydrophobic (or hydrophilic) mixing ratio-dependent pKa variation of the carboxyl group. Interestingly, we observed a counterintuitive, non-monotonic behavior that a fractionally mixed hydrophobic group can induce significant enhancement of dielectric strength of the interfacial water. In particular, such a fractional mixing substantially decreases the amide coupling efficiency at the surface, as manifested by the corresponding pKa decrease. The SERS-based platform we demonstrated can be widely applied for atomically precise control and molecular-level characterization of hydration water on various heterogeneous surfaces of biological and industrial importance.

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 10:12

Chair: Han-Kyu Choi (Kunsan National University)

Improving Empirical Density Functionals via DC-DFT

Suhwan Song, Eunji Sim^{*}

Department of Chemistry, Yonsei University, Korea

All Kohn-Sham DFT calculations with approximate functionals have energy errors from two distinguishable sources: the error in the XC energy and the error in the self-consistent density. These two different sources of error interfere with the standard empirical fitting process, especially if the signs are different. We illustrate this danger with stretched H_2^+ system, which can explicitly perform error decomposition. However, this issue can be predictable and avoidable by performing the usual fitting process only for Functional error based on the DC-DFT scheme. We show that a simple double-hybrid, applied only to Hartree-Fock densities, yields remarkable accuracies on various chemical databases.

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 10:20

Chair: Han-Kyu Choi (Kunsan National University)

Substructure-based neural machine translation for retrosynthetic prediction

Umit Volkan Ucak, Juyong Lee^{1,*}

chemistry, Kangwon National University, Korea

¹*Department of Chemistry, Kangwon National University, Korea*

With the rapid development of the modern computational retrosynthetic planning techniques, machine translation architectures, including neural machine translation have started to play an important role in finding reasonable synthetic pathways for a target molecule. Theoretical findings suggest that linguistic-analysis are readily be applied to find solutions to problems of chemical linguistic. Therefore, retrosynthetic planning can be appropriate for the sequence-to-sequence frameworks of neural machine translation. In this work, we recast the retrosynthetic planning problem as a language translation problem by using a template-free sequence-to-sequence model, trained end-to-end and fully data-driven. Unlike models translating between the SMILES strings of reactants and products, we introduce a new way of representing a chemical reaction based on molecular fragments. The new approach resolves major drawbacks of existing retrosynthetic methods such as invalid SMILES problem. With this approach, we demonstrate better prediction results than current state-of-the-art computational methods. Specifically, our approach predicts bio-actively similar reactant molecules with an accuracy of 57.7%.

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

Oral Presentation for Young Physical Chemists

Room 404 (Live Streaming) THU 10:28

Chair: Han-Kyu Choi (Kunsan National University)

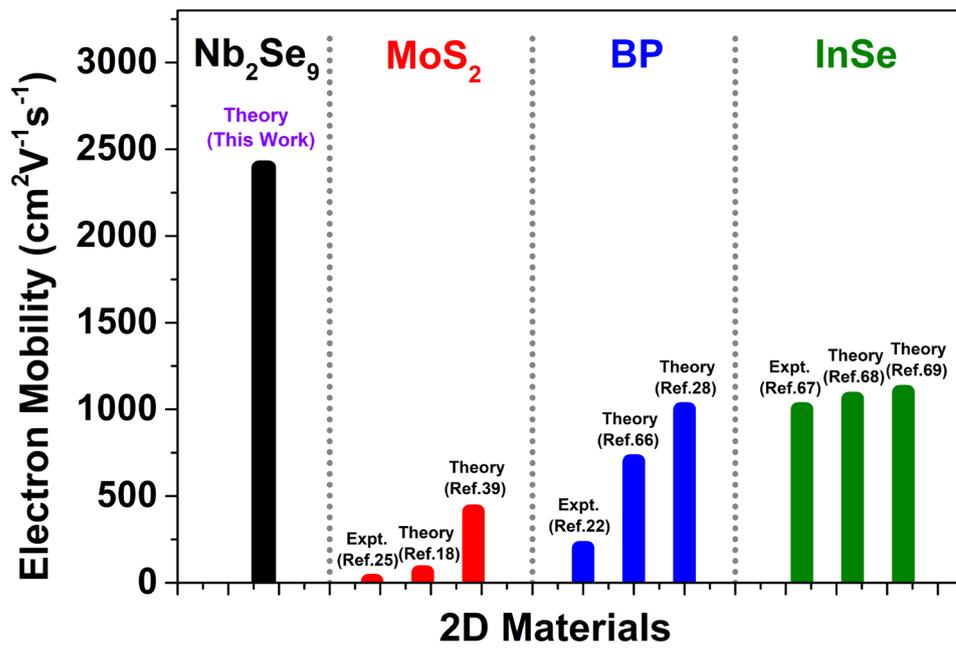
Effect of dimensionality in anisotropic transport behavior for van der Waals Nb₂Se₉ chain structures

You Kyoung Chung, Junho Lee¹, Joonsuk Huh^{1,*}

Department of Chemistry, SungKyunKwan University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

We investigated the charge transport of vdW Nb₂Se₉ chain structures with semiconductor properties by dimensional reduction from bulk to a single nanowire (SN). On the basis of the deformation potential (DP) theory, our theoretical calculations showed that the reduction of dimension affects the effective mass, deformation constant, and elastic constant of mobility anisotropy of Nb₂Se₉ materials. We found that the electron mobility values of the 2D_(010) planes are $1.74 \times 10^3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ (calculated with the PBE-D3 functional) and $2.40 \times 10^3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ (calculated with the HSE06 functional) along a direction when anisotropic parameters are used, whereas the hole mobility values for bulk Nb₂Se₉ at room temperature are $1.19 \times 10^2 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ (PBE-D3) and $1.18 \times 10^2 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ (HSE06). Thus, the electron mobility of the 2D structure along the **a** axis is 20-100 times greater than the hole mobility of the bulk structure. Our band-decomposed partial charge analysis showed that the high electron mobility of the 2D plane of Nb₂Se₉ originates from the high charge distribution and large orbital overlap. We expect that the 2D Nb₂Se₉ material can be used as a p-type semiconductor in optoelectronic and thermoelectric nanodevices because of its high electron mobility, suitable bandgap, and dangling-bond-free character.



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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:00

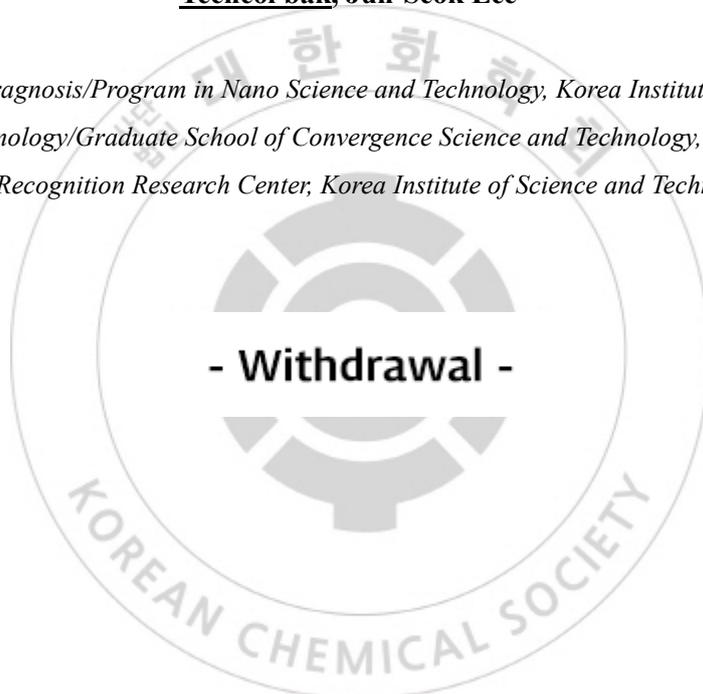
Chair: Donghoon Han (The Catholic University of Korea)

**[Withdrawal] A Rapid and simple electrochemiluminescence method
for analysis of the hydrogen sulfide level in the blood**

Yecheol bak, Jun-Seok Lee^{1,*}

*Center for theragnosis/Program in Nano Science and Technology, Korea Institute of Science and
Technology/Graduate School of Convergence Science and Technology, Korea*

¹Molecular Recognition Research Center, Korea Institute of Science and Technology, Korea



- Withdrawal -

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:09

Chair: Donghoon Han (The Catholic University of Korea)

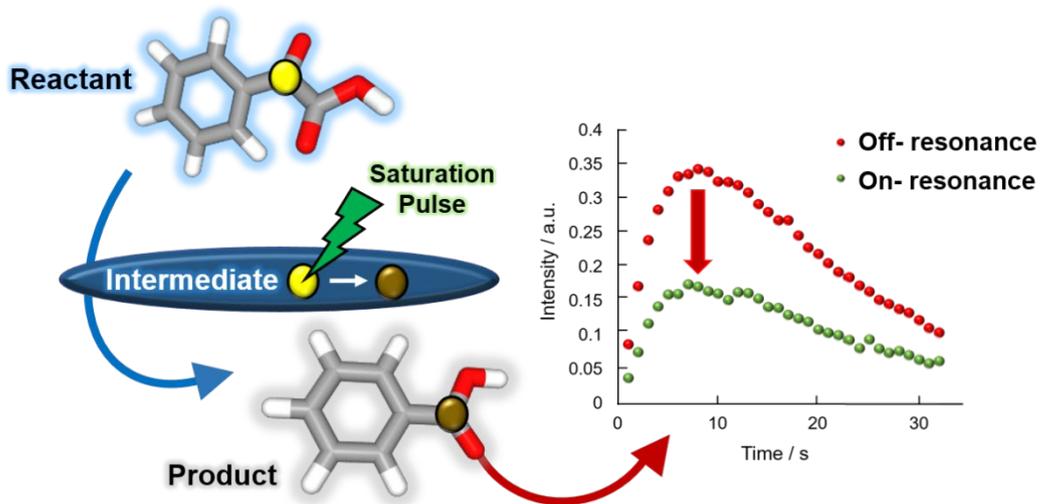
Invisible reaction intermediate studies in decarboxylation reaction of phenylglyoxylic acid and hydrogen peroxide by blind saturation using D-DNP

Jiwon Kim, Youngbok Lee^{1,*}

Department of Bionano technology, center for Bionano Intelligence Education and Research , Korea

¹*Department of Bionano technology, Department of Applied chemistry, Korea*

D-DNP (Dissolution-dynamic nuclear polarization) technique can enhance NMR signal by several orders of magnitude, allowing NMR spectroscopy to investigate reaction mechanisms and kinetics in real time. However, in preliminary mechanism studies using D-DNP, reaction intermediates with a sufficiently high stability and population during the NMR measurement time were observable. Here, we conducted blind saturation experiments using D-DNP to demonstrate whether invisible intermediates of unlabeled compounds can be identified in decarboxylation reaction between α -keto acid and hydrogen peroxide. First of all, a prior study using $1,2\text{-}^{13}\text{C}$ pyruvate was carried out and it was observed that the product signal decrease as applying a selective saturation pulse to the intermediate of pyruvate. Subsequently, phenylglyoxylic acid (PHGA) was used to conduct a "wide" selective saturation experiment, showing that the reaction intermediate of PHGA is present in a region of 99 to 105 ppm similar to pyruvate. To acquire more accurate chemical shift information of PHGA intermediate, a "narrow" selective saturation experiment was proceeded and the pulse was applied at an excitation range of 1 ppm while changing the frequency center within 99 to 105 ppm. As a result, it was possible to determine the chemical shift information about intermediate of PHGA, observing that the intensity of product was significantly reduced when selective saturation is applied at 103 ppm. In conclusion, we successfully obtained the chemical shift of reaction intermediate not visible in NMR spectrum through blind selective saturation method which is expected to be effectively used to identify important and complex chemical and biological pathways.



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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:18

Chair: Donghoon Han (The Catholic University of Korea)

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

Sang Tak Lee, Han Bin Oh*

Department of Chemistry, Sogang University, Korea

The outbreak of the SARS coronavirus 2 (SARS-CoV-2) pandemic has deeply affected every aspect of our lives. Especially, the use of disinfecting products increased explosively to prevent the virus transmission and to guarantee the sanitization of personal and public hygiene. Among the different active ingredients used in the disinfectants, quaternary ammonium compounds (QACs) are the most intensively used material. QACs have been widely used in the consumer chemical products (CCPs) such as personal hygiene, cosmetics, detergents, fabric softeners, eyedrops, etc. Almost 1 million pounds of QACs are produced annually and resulting residual QACs in various environmental, food and dust samples are detected. As the QACs are more intensively used in households, the exposure assessment of the QACs introduced by different routes should be carried out. In this research, an analytical method using liquid chromatography tandem mass spectrometry (LC-MS/MS) was applied to identify and quantify 3 different QACs in CCPs. To carry out the exposure assessment, the guidelines suggested by the US Environmental Protection Agency (US EPA) and Korea Ministry of Environment were followed to specify the exposure routes and scenarios. Particularly, two specific routes, the oral ingestion and dermal contact, were investigated to estimate how much QACs a person is exposed to while using CCPs. For the percutaneous permeation study of QACs, the Franz cell and skin-like membrane were utilized to quantify the amount of QACs penetrated the skin. From the exposure amount determined for each route and scenario, the overall risk assessment of the QACs in the CCP could be estimated.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:27

Chair: Donghoon Han (The Catholic University of Korea)

Facile Synthetic Methods of Magnetic Carbon Nanoparticles with Different Morphological Features and its Application on Adsorption / Adsorption Mechanism of Organic Substances

Quy Son Luu, Uyen Thi Do, Jiwon Kim, Donghyeok Jo, Thi Quynh Nguyen, Youngbok Lee*

Department of Bionano Technology, Center for Bionano Intelligence Education and Research, Hanyang University, Korea

Magnetic carbon nanomaterials were used extensively as an adsorbent in the last two decades due to high surface area and easy recovery. Herein, we present a comparison of three magnetic carbon nanosphere (MCNs), which are synthesized from polydopamine (PDA) and iron or iron oxide nanoparticles (Fe₃O₄ NPs) for adsorption methylene blue (MB). Three MCNs are prepared with similar size (~200 nm) and spherical morphology, including multi-core, core-shell, and linker structures. Many previous studies utilized the multi-core and core-shell structure in their reports, the linker is new material in our research. It is designed by carboxylic acid-functionalized activated carbon nanospheres (ACNs-COOH) connected with amine-terminated iron oxides NPs (Fe₃O₄-NH₂) through the carbodiimide crosslinking reaction. Therefore, linker material is shown the highest specific surface area and strong magnetism. Because of this reason, the linker sample exhibits the highest maximum adsorption capacity based on the Langmuir isotherm model at pH=10 for removal MB; and it can separate easily by an external magnetic field. Moreover, we proposed the adsorption mechanism of three MCNs through electrostatic interaction, π - π interaction, and intraparticle diffusion kinetic model.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:36

Chair: Donghoon Han (The Catholic University of Korea)

Development of an universal method for simultaneous analysis of 46 neurotransmitters in mouse brain cell culture medium, tissue lysate and serum using liquid chromatography coupled to tandem mass spectrometry

Nu Ri Lim, Ki Hun Kim*

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

Neurotransmitters play an important physiological role in the body, which have been associated with diseases. Therefore, accurate measurement of neurotransmitters in diverse matrices is essential as it can provide a procedure for diagnosing and treating diseases. In this study, we developed and optimized the rapid simultaneous analytical method for multiple neurotransmitters remaining in fetal mouse brain cell culture medium, brain tissue lysate and mouse serum using liquid chromatography coupled to tandem mass spectrometry. We optimized analytical methods for 46 target neurotransmitters and their metabolites to improve the reproducibility and accuracy of the benzoyl chloride derivatization preparation process. We focused to optimized benzoyl chloride concentration, derivatization temperature and reaction time for high sensitivity and the values were that 0.5%, 1 °C and 10 minutes, respectively. Furthermore, pH (9.6 with carbonate-bicarbonate buffer) was also critical factor, and we observed an increase in sensitivity for Adenosine (684.7%), 3-methoxytyramine (112.6%), Spermidine (72.5%), Serotonin (41.1%), Tyramine (57.0%), Dopamine (35.3%) and Epinephrine (22.5%) compared to using sodium carbonate solution. The method with derivatization of samples was validated. Linearity was obtained ($R^2 \geq 0.98$) and the intra and inter-day precision of the method were ranged from 9.6% to 24.0%. The accuracy of the method was 85.0~114.6%. The developed method could be suitable for rapid analyzing neurotransmitters in various matrices.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:40

Chair: Donghoon Han (The Catholic University of Korea)

Effective Sample Preparation and determination of nicotine enantiomer in E-Liquid using Dispersive Liquid-Liquid Microextraction HPLC-UV

Seung Hoon Song, Seung Woon Myung*

Department of Chemistry, Kyonggi University, Korea

In this study, the contents of (S)-(-)-nicotine and (R)-(+)-nicotine were analyzed for various types of nicotine after efficiently extract the enantiomeric nicotine present in E-Liquid using dispersive liquid-liquid microextraction(DLLME). In order to optimize DLLME, experiments were conducted on the pH, extraction solvent, dispersive solvent, and type and amount of salt. The LOD of chiral nicotine was 0.11 µg/mL and 0.17 µg/mL, respectively, and the LOQ was 0.3 µg/mL, 0.44 µg/mL, It was confirmed through an experiment. The calibration curve was designed to be 0.3 – 18 µg/mL, 0.44 – 4.4 µg/mL, respectively, and the correlation coefficient (r^2) was 0.9978 – 0.9996. As a verification of the optimized method, accuracy and precision were measured by dividing it into intra-day and inter-day. In the experiment conducted with intra-day, accuracy was 79.9-110.6%, and the precision was 1.3-12.0%. In the inter-day, accuracy was 87.8 – 108.0%, and the precision was 4.0 – 12.8%. This analysis of chiral nicotine using DLLME uses less organic solvents than LLE method and is an excellent method that allows sample preparation within a short time.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:44

Chair: Donghoon Han (The Catholic University of Korea)

Rapid and visual detection of folic acid using paper-based analytical devices

DaeHyun Kwon, Nguyen Ngoc Nghia¹, Bui The Huy¹, Yong-Ill Lee^{1,*}

Department of chemistry, Changwon National University, Korea

¹*Department of Chemistry, 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-Cu²⁺ (RhB-Cu²⁺) as a color indicator. The color intensity of RhB-Cu²⁺ was enhanced significantly after adding analyte. It can be explained by the improvement of electron transfer from RhB-Cu²⁺ 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.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:48

Chair: Donghoon Han (The Catholic University of Korea)

Single Particle Study: Plasmonic Damping Induced by Mercury Amalgamation in Anisotropic Gold Nanorods

Geun Wan Kim, Ji Won Ha*

Department of Chemistry, University of Ulsan, Korea

Amalgamation is a concentrating process in which metallic gold or silver is mixed with mercury (Hg). Herein, we investigated the plasmon damping of single gold nanorods (AuNRs) caused by mercury amalgamation. First, the time-dependent structural change and the formation of Hg-Au alloy nanorods were studied by scanning electron microscopy (SEM). The aspect ratio of AuNRs decreased due to the mercury amalgamation that resulted in the structural change from a rod to a sphere shape. Second, scattering-based dark-field (DF) microscopy and spectroscopy are powerful tool to characterize optical properties of plasmonic nanoparticles at the single particle level. Thus, in this study DF microscopy and spectroscopy was used to gain new insight into the optical properties and plasmon damping of the Hg-Au alloy nanorods at the single particle level. A strong plasmon damping (or linewidth broadening) in the scattering spectra of single Hg-Au alloy nanorods was observed due to the formation of mercury amalgamation on the AuNR surface. Furthermore, the results indicate that the plasmon damping in single AuNRs can be used as a promising strategy for mercury sensing.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:52

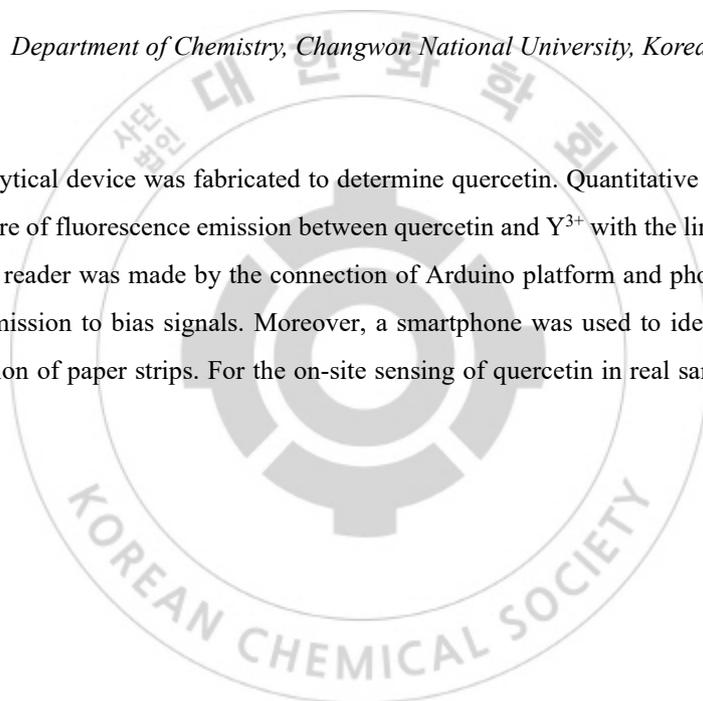
Chair: Donghoon Han (The Catholic University of Korea)

Quercetin sensor using paper-based analytical devices

Nguyen ngoc Nghia, Bui The Huy, Yong-Ill Lee*

Department of Chemistry, Changwon National University, Korea

A paper-based analytical device was fabricated to determine quercetin. Quantitative analysis of quercetin based on the measure of fluorescence emission between quercetin and Y^{3+} with the limit of detection of 27 nM. A home-made reader was made by the connection of Arduino platform and photodiode to transduce the fluorescence emission to bias signals. Moreover, a smartphone was used to identify hue value from fluorescence emission of paper strips. For the on-site sensing of quercetin in real samples, this technique could be used.



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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 09:56

Chair: Donghoon Han (The Catholic University of Korea)

Analysis of Hydrotreated and Untreated Atmospheric Residue Oil by Atmospheric Pressure Photoionization Cyclic Ion Mobility and ultrahigh-resolution mass spectrometry

Eunji Cho, Sunghwan Kim^{1,*}

Mass Spectrometry based Convergence Research Institute, Kyungpook National University, Korea

¹Department of Chemistry, Kyungpook National University, Korea

Since crude oil is composed of many compounds within a narrow mass range, ultrahigh resolution mass spectrometry (UHR-MS) is basically an important analytical tool. UHR-MS such as Fourier transfer ion cyclotron resonance mass spectrometer (FT-ICR MS) is an obvious choice to determine the chemical compositions of crude oil, but identifying structural isomers is limited because they cannot be separated. In this study, cyclic ion mobility mass spectrometry (CIM-MS) was combined to enable structural analysis of compounds in crude oil. Atmospheric residue samples before and after hydrotreating process were compared. Samples prepared at 0.5mg/mL in toluene were analyzed in positive atmospheric Pressure Photoionization coupled to CIM and FT-ICR MS. When the drift time obtained from CIM-MS was compared, there was a significant difference between the samples with and without hydrotreating process. The widening of the peak width of the drift time (DT) means that there are many isomers of the compound. The higher the double bond equivalent (DBE), the wider the DT width was observed. As the DBE increased, the structure isomers were also increased. Understanding the structural change occurred by the chemical process is very important because it greatly affects recovery of high-quality petroleum generated during the process. Therefore, the analytical methods shown in this study can provide pivotal platform to study structural changes occurred during hydrotreating of oils.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:00

Chair: Donghoon Han (The Catholic University of Korea)

Chiral analysis with helical magnetic field induced chiral plasmonic sensor

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Analysis of chiral analytes from small size monomers to large size polymers with chirality has been challenged for effective chiral sensing of drug safety of pharmaceutical. We already have introduced chiral sensing which chiral-active magnetoplasmonic nanoparticles (MNPs) were assembled into helical nanochain structure in helical magnetic field (hB). Ag@Fe₃O₄ core-shell NPs were used for sensing materials that are aligned by a magnetic field. Helically aligned MNP showed remarkable circular dichroism and lead to enhance the CD signals at lower concentration than the technical limit of detection (LOD). This enhancement has successfully occurred in monomers, polymers, and drugs. When left and right polarized light interacted with chiral molecule in hB system, the notable changes of the circularly irradiated light was appeared. Also, different aspects of enhanced signals were observed depending on the type of amino acid. This hB induced chirality enhancer can lead to qualitative and quantitative analysis, which is expected to be applied to the pharmaceutical and biological sensing fields.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:04

Chair: Donghoon Han (The Catholic University of Korea)

SERS-based aptasensor for the rapid classification of influenza A & COVID-19 viruses

Hao Chen, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

The ongoing Coronavirus disease 2019 (COVID-19), caused by severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2), has a clear potential for a long-lasting global pandemic, high fatality rates, and incapacitated health systems. More than 100 million cases of Covid-19 have been reported worldwide, including over 2.4 million deaths. Meanwhile, influenza A is also widely spread globally, which has similar symptoms but causes fewer morbidity and mortality. Reverse transcription-polymerase chain reaction (RT-PCR) is the critical diagnostic technique being used. This diagnostic method delivers results with good sensitivity and excellent specificity but is expensive and is slowed by transport to testing laboratories. We aim at designing an aptasensor for inexpensive, simple, rapid diagnostics of SARS-CoV-2 and influenza antigens at the early stage of the disease. Our group has recently developed a SERS-based aptasensor to perform a rapid and sensitive influenza A virus assay. Inspired by our previous work, a dual SERS-based assay platform for the detection of SARS-CoV-2 and influenza A antigens was developed. Herein, a 3D nanopopcorn plasmonic substrate was fabricated using the surface energy difference between a perfluorodecanethiol (PFDT) spacer and the Au layer. Quantitative evaluations of SARS-CoV-2 and influenza virus antigens were performed using a decrease in Raman intensity due to the release of two specific Raman reporter-labeled DNA aptamers from nanopopcorn substrate surfaces via interactions between aptamers and virus proteins. We expect this aptasensor platform to provide new insight into developing a novel platform for rapid classification of COVID-19 and influenza A.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:08

Chair: Donghoon Han (The Catholic University of Korea)

LC/MS-based polar metabolites analysis after axon regeneration in peripheral nerve-injured mouse

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Western Seoul Center, Korea Basic Science Institute, Korea

Peripheral nerve damage causes severe sensory and motor dysfunction. However, after peripheral nerve injury, axon regenerate and function is restored. Therefore, the process of axon regeneration after nerve injury is important and metabolic studies are needed. We observed changes in polar metabolites of axon regeneration in nerve-injured mouse. In this study, we performed the non-targeted polar metabolomic profiling of dorsal root ganglion (DRG) tissue from mouse using ultra performance liquid chromatography/quadrupole time of flight mass spectrometry (UPLC/Q TOF MS). 10 control mice and 10 nerve-injured mice with regenerated axons after sciatic nerve crushing were analyzed. Multivariate analysis showed discriminated metabolic pattern between control group and nerve injury group. Non-parametric t-test was used to find significantly different metabolites between control group and nerve-injured group. As a result, glutathione, histamine, N-acetylaspartate, creatinine, N-acetylaspartylglutamic acid, D-fructose 6-phosphate significantly decreased, whereas glutathione oxidized, leucine, glutamate, histidine, phenylalanine, glutamine, uridine, UDP-N-acetylglucosamine significantly increased after nerve-injured mice. Pathway analysis revealed that significant metabolic pathway were glutathione metabolism, alanine, aspartate and glutamate metabolism and histidine metabolism in nerve-injury mice. These results showed that polar metabolites were changed after axon regeneration in nerve-injured mouse compared to control. This study demonstrates that the LC-MS based non-targeted polar profiling can be a used to understand the mechanism of axon regeneration in peripheral nerve-injured mouse.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:12

Chair: Donghoon Han (The Catholic University of Korea)

Enhanced Signal Boosts of Silicon Nanoparticles via Selective ^{29}Si Isotope Enrichments for DNP-MRI Applications

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Nuclear Magnetic Resonance (NMR) spectroscopy is one of the principal analytical tools for biological applications since the method provides structural information and molecular interactions. However, due to severe sensitivity issues originated from both low magnetic moments and low natural abundance of NMR active nuclei, except hydrogen atom, there are many restrictions conducting NMR experiments in general conditions. Dynamic Nuclear polarization (DNP) is one of the strong tools to enhance the sensitivity of the NMR signal by transferring the high polarization level of electron spins to low polarization level of nuclear spins using microwave irradiation. Another powerful tool is isotope enrichment, which is the most direct way to increase the signal by increasing the amount of NMR active nuclei. In this research, we experimented by applying these two methods to silicon nanoparticles. A DNP experiment was proceeded by synthesizing particles having 10% and 15% ^{29}Si nanoparticles based on the 4.67% silicon nanoparticle, which is the natural abundance of silicon. To determine the effect of enrichment, the signal of enriched silicon nanoparticles is measured in DNP-NMR, and the build-up constant and T1 relaxation time are calculated through build-up and decay test. After that, the MRI phantom image is measured to make sure whether the signal amplification by DNP is detected within the MRI. Finally, the possibility as an imaging agent is confirmed through an in vivo experiment using a mouse. This research is expected to contribute examining effect of enriched-silicon as potential molecular imaging probes.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:16

Chair: Donghoon Han (The Catholic University of Korea)

Synthesis and characterization of LiMBO_3 as a cathode material for lithium secondary batteries

HyeSeung Kwon, Youngil Lee^{1,*}

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

Researches on polyanionic structured lithium metal borate material, LiMBO_3 ($M = \text{Mn, Fe or Co}$), as a cathode material for lithium secondary batteries have been actively conducted due to its light weight, structural stability, and high theoretical capacity (220 mAh g⁻¹). Herein, $\text{LiMn}_{1-x}\text{Co}_x\text{BO}_3$ and $\text{LiFe}_{1-x}\text{Co}_x\text{BO}_3$ ($x = 0, 0.25, 0.5, 0.75, \text{ and } 1.0$) have been synthesized by sol-gel method. To characterize the crystal structure and microstructure, X-ray diffraction (XRD) and solid phase ⁷Li MAS NMR spectroscopy have been measured. In addition, via Galvano static charge/discharge test, oxidation/reduction potentials and operating voltage have been studied. Quantitative analysis for chemical composition of materials has been also performed with laser induced breakdown spectroscopy (LIBS).

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:20

Chair: Donghoon Han (The Catholic University of Korea)

Site-specific TEMPO mediated FRIPS for a model protein using genetically incorporated unnatural amino acid: Structure dependent radical dissociation of protein

Jae-ung Lee, Hyunsoo Lee*, Han Bin Oh*

Department of Chemistry, Sogang University, Korea

The radical driven dissociation using TEMPO mediated FRIPS is a powerful approach for peptide sequencing under collisional activation. It provides efficient analysis of peptides having disulfide bonds or post-translation modifications like other radical based techniques because fragmentation mechanism follows nonergodic process. However, the previous method has a limitation in introducing the TEMPO based reagent at a desired site because the conjugation unit, -NHS functional group, can only conjugates with primary amines, generally only with N-terminal amine after blocking lysine residues. In this study, we suggested the site-specific TEMPO mediated FRIPS for protein structure analysis using genetically incorporated unnatural amino acid, where one of the residues in model protein (affibody) was modified to acetylphenylalanine, followed by the conjugation of modified TEMPO based reagent. We chose multiple modification/conjugation sites considering the three-dimensional structure, and the tandem mass spectrometry experiments were conducted. The results showed that the sites of radical driven fragmentation were closely related to the modification/conjugation sites. We are conducting additional experiments to obtain clear relationship between the radical position and protein structure by differing the modification/conjugation sites. We anticipate that this approach could provide a new way to the elucidation of protein structure.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:24

Chair: Donghoon Han (The Catholic University of Korea)

Effect of the enhanced hydrophobic effect on structured and unstructured proteins in D₂O and H₂O.

MyungKook Son, Chae Ri Park, Sooyeon Chae, Dongjoon Im, Dongvin Kwak, Hugh I.

Kim *

Department of Chemistry, Korea University, Korea

To avoid spectroscopic peak interferences such as H resonance frequency or O-H vibrational frequency in nuclear magnetic resonance (NMR), infrared (IR) spectroscopy etc., deuterium oxide (D₂O) is used as a solvent for a deuteration of sample molecules. Deuteration is used to avoid spectroscopic interferences, but it is controversial whether deuteration influences protein structures. Deuterium oxide (D₂O) is used at nuclear magnetic resonance (NMR), infrared (IR) spectroscopy as a solvent to avoid peak interferences, such as H resonance frequency or O-H vibrational frequency. Due to lower vibrational frequency of O-D (~1200 cm⁻¹) than that of O-H (~1600 cm⁻¹), D₂O is more stable than H₂O, with stronger hydrophobic effect. For this reason, there was a research that a globular protein is more stable in D₂O. But there is few researches about the protein structural changes or protein fibrillation mechanisms in D₂O. In this research, we used human insulin and α-synuclein to study the effect of reinforced hydrophobic effect on the structured proteins and IDPs' structures and protein stability-fibrillation. In addition, the experiment was further carried out under conditions of structural denaturation by adding sodium dodecyl sulfate (SDS), a protein denaturant, to insulin. 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-18**

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:28

Chair: Donghoon Han (The Catholic University of Korea)

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

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

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

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:32

Chair: Donghoon Han (The Catholic University of Korea)

Comparison of thermal desorption (TD) sorbent tubes with SPME fibers for the analysis of combustion gases from fossil fuels

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The characterization of combustion gases from fuel oils is important for the identification of cause of fire and investigation of arson suspects. In this study, we combusted three kinds of fuel oils such as diesel, kerosene, and gasoline refined by three different refinery companies, for which combustion gases were characterized using TD/GC-MS and SPME/GC-MS. For the comparison purposes, two TD sorbent tubes (Tenex® TA, and Airtox™) and four SPME fibers (PDMS, PDMS/DVB, CAR/PDMS, and DVB/CAR/PDMS) were utilized for gas sampling. The results showed that two different sampling methods have comparable absorption efficiencies. In addition, three different TD sorbent tubes and fibers showed different compatibility to the type of fuel oils. It was found that Airtox™, CAR/PDMS, and DVB/CAR/PDMS are suitable for the adsorption of combustion gases from kerosene and diesel. Tenex® TA and CAR/PDMS showed high adsorption compatibility for gasoline. On the other hand, Airtox™ was found to be the most appropriate adsorption tube for relatively light gases under 130 Da.

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

Oral Presentation of Young Analytical Chemists I

Room 301 (Live Streaming) THU 10:36

Chair: Donghoon Han (The Catholic University of Korea)

Investigating the deteriorated drug efficiency of cisplatin induced by DMSO using ICP-MS

Dongvin Kwak, Hugh I. Kim^{*}, Sooyeon Chae, MyungKook Son, Dongjoon Im, Chae Ri Park

Department of Chemistry, Korea University, Korea

Cisplatin (cis-[Pt(NH₃)₂Cl₂]) is a platinum-based anticancer drug used for diverse cancers. Because of acquired or intrinsic resistance against to cisplatin, a large number of in vitro studies have been conducted to clarify the mechanism of this phenomena. In most of these studies, dimethyl sulfoxide (DMSO) has been utilized as solvent for the stock solution of cisplatin. According to a study concerning effects of solvents on the activity of cisplatin, DMSO depresses cytotoxic efficiency via ligand exchange with Cl⁻. However, very few studies have been published on which steps DMSO affects on. The steps is divided into 1. Passive diffusion/transportation through cell membrane/transporters 2. One or two Cl⁻ ligands are exchanged with H₂O due to low [Cl⁻] in cytoplasm resulting active form 3. Active forms of cisplatin coordinate mainly to N(7) of guanine, adenine 4. DNA kink induced by Pt coordination leads cell apoptosis signalling pathways. In this study, we investigated which steps exactly are affected by DMSO solvent.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 10:40

Chair: Ki Hun Kim (KIST)

In situ Analysis of Cocaine Metabolites in Fresh and Aged Dried Blood Spots

Ayoung Kim^{*}, Jim Reynolds^{*}

Department of Chemistry, Loughborough University, United Kingdom

Urine and blood testing are widely used to detect drugs and their metabolites in biological fluids, and this can be useful in a forensic investigation to examine criminal evidence. However, biological samples like urine and blood can have problems associated with their analysis, for example, biological fluids and any environmental contaminants provide a complex sample matrix which frequently requires lengthy clean-up and separation steps. In this research Sheath-Flow Probe Electrospray Ionisation (sfPESI) was interfaced with mass spectrometry as a direct analysis method to analyse dried blood spots for drug metabolite analysis in situ. sfPESI is a minimally destructive method and was mainly coupled to a Thermo Exactive Orbitrap mass spectrometer to enable sample analysis under ambient conditions, with no requirement for prior sample preparation. Samples were taken by touching the dried blood spots with the sfPESI needle for 5 to 10 seconds to allow solvent extraction. 50% ethanol:water solution containing 0.5mM sodium acetate and 0.1% formic acid used as the extraction solvent for the sfPESI probe. 2.5 kV voltage was applied to the sfPESI emitter for 5 seconds to facilitate an electrospray, by pulsing the voltage applied to the sfPESI emitter a rapid separation of the metabolites from background species can be achieved, enhancing the metabolites mass spectral response. sfPESI-MS was applied to measure the cocaine metabolites, benzoylecgonine (BZE), ecgonine methyl ester (EME), and Cocaethylene (CE), in dried blood spots. The metabolites were spiked into whole blood at a range of concentrations from 0.1 to 10 $\mu\text{g}/\text{mL}$. 5 μL blood of each mixture were deposited onto glass microscope slides or filter paper and allowed to dry. For ageing experiments samples were stored in a dark cupboard at 20 $^{\circ}\text{C}$ for up to 1 year. Protonated and sodiated cocaine metabolites could be detected reliably in dried blood spots at levels down to 0.5 $\mu\text{g}/\text{mL}$. Additionally, the cocaine metabolites and other constituents in the dried blood spots such as lipids could be detected after a year of dried blood spots ageing. The method shows a semi-quantitative response over the range of 0.5 – 10 $\mu\text{g}/\text{mL}$ ($R^2=0.9604$) with a RSD precision of 28% ($n=10$) at the 1 $\mu\text{g}/\text{mL}$ level in

benzoylecgonine (BZE) analysis. These data demonstrate the potential of sfPESI-MS to rapidly identify a drug metabolite in fresh and aged dried blood spots at physiologically relevant levels.



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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 10:50

Chair: Ki Hun Kim (KIST)

Inkjet-based microreactor for the synthesis of silver nanoparticles on plasmonic paper decorated with chitosan nano-wrinkles for efficient on-site surface-enhanced Raman scattering (SERS)

Truong Thi thuy, Sharipov Mirkomil¹, Bui The Huy¹, Yong-Il Lee^{1,*}

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¹*Department of Chemistry, Changwon National University, Korea*

Here we report a synthesis approach that is simple, surfactant free, and green, and which is additionally cost effective in terms of its material requirements. The approach entails the use of an inkjet microreactor for the deposition of silver nanoparticles on the surface of office paper decorated with chitosan nano-wrinkles for the preparation of a reproducible and sensitive paper-based surface-enhanced Raman scattering (SERS) 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 (AA). Pre-modification of the paper with chitosan allowed the formation of randomly oriented nano-wrinkles on the surface, thus enabling the formation of silver nanoparticles with good hotspots. The novel paper-based SERS substrate showed outstanding sensitivity and spot-to-spot reproducibility for on-site detection using a portable Raman spectrometer with a limit of detection (LOD) of 10.7 pM. Moreover, our paper-based SERS substrate has an excellent enhancement factor (EF) of 7.4×10^8 , which is difficult to achieve on a paper substrate because of the microporous nature of paper. Finally, the batch-to-batch reproducibility and long-term stability of the SERS substrate under ambient conditions make this substrate a good candidate for point-of-care test (POCT) applications.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 10:54

Chair: Ki Hun Kim (KIST)

Development of a portable SERS-based lateral flow assay system for on-site diagnosis of SARS-CoV-2

Younju Joung, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

SARS-CoV-2 has spread globally to more than 200 countries, and more than 100 million cases of SARS-CoV-2 have been reported worldwide. A rapid and accurate test for SARS-CoV-2 is urgently needed to control the spread of the viruses. Reverse transcription-polymerase chain reaction (RT-PCR) has been considered a gold standard for detecting SARS-CoV-2 target genes. In RT-PCR, however, the total diagnostic time, including sample preparation, gene amplification, and detection, takes approximately 3-4 hours. Thus, it is necessary to shorten the diagnostic time for rapid on-site diagnosis. Various rapid kits for immunodiagnosis using antigen-antibody reactions were also developed to shorten the diagnosis time. However, they have not been adopted as the standard diagnostic method due to their low accuracy. In particular, the “false-negative” problem of commercialized immunodiagnostic kits is recognized as a severe problem that can aggravate the spread of the SARS-CoV-2. To resolve the issues, we have developed a SERS-based lateral flow assay (LFA) sensor with a portable Raman reader for rapid and sensitive immune analysis of SARS-CoV-2. We believe that the portable SERS-based LFA sensor enables on-site diagnostics of SARS-CoV-2. The quantitative evaluation of SARS-CoV-2 in a transport medium solution containing nasopharyngeal swabs is possible. Our SERS-based LFA sensor shows a strong potential to resolve the problems in terms of low sensitivity and limit in quantitative analysis inherent in conventional antigen tests to detect SARS-CoV-2.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 10:58

Chair: Ki Hun Kim (KIST)

^1H NMR-based metabolomic profiling to identify the treatment effect of acupuncture in patients with functional dyspepsia

Heeyeon Lee, Geum-Sook Hwang*

Korea Basic Science Institute, Korea

Functional dyspepsia (FD) is a common functional gastrointestinal disorder in clinical gastroenterology with multiple pathogenic mechanisms. Many possible factors including abnormal neurohormonal function, autonomic dysfunction, visceral hypersensitivity or mechanical distention, psychosocial comorbidity and stress are to be considered in the pathogenesis of FD. Acupuncture, an important therapeutic method based on meridian theory in traditional Chinese medicine, has been shown to be effective for the manipulation of abnormal physiological conditions in the human body and for the treatment of various functional diseases such as FD. However, there are few metabolic studies relevant to the treatment effect of acupuncture in FD patients. In this study, we analysed urinary and serum metabolites to investigate the treatment effects of acupuncture in FD patients. We performed metabolic profiling using nuclear magnetic resonance (NMR) spectroscopy to investigate metabolites in urine and serum samples from patients with FD. Several metabolites were significantly changed in urine and serum sample of FD patients who received acupuncture treatment, and it was confirmed that specific metabolite could be a marker proving effective acupuncture treatment in FD patients. This study demonstrates that the urinary and serum metabolites of FD patients were changed after acupuncture treatment, and metabolomics approach can be used to investigate the treatment effects of acupuncture in FD patients.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:02

Chair: Ki Hun Kim (KIST)

The Efficacy of Antibacterial Feed to evaluate Bacterial Diseases Resistance in *Paralichthys Olivaceus*

Junghoon Kang, Miseon Jeong, Youngjin Kim, Wonryeon Cho*

Department of Chemistry, Wonkwang University, Korea

In the previous study, the efficacy of antibacterial feed was analyzed by detecting the protein expression of *Paralichthys olivaceus* (*P. olivaceus*) before and after feeding the antibacterial feed. After feeding antibacterial feed for 4 weeks, this study further intends to analyze the disease resistance by detecting the protein expression of *P. olivaceus* which was artificially infected with *Streptococcus iniae* (*S. iniae*). Among the bacterial diseases, *S. iniae* is known to infect many fish species and is therefore, an important causative agent of streptococcosis in *P. olivaceus* culture. Proteins were extracted with RIPA buffer from homogenized head kidney tissues of *P. olivaceus*. Each supernatant fluid was pooled into three groups according to time period after artificial infection. Pooled samples from *P. olivaceus* were trypsin digested and desalted. After that, the proteins in three groups were analyzed with nLC-MS/MS and protein database searches. The disease resistance as efficacy of the antibacterial feed was evaluated with differentially expressed protein (DEP) and gene ontology (GO) enrichment analysis.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:06

Chair: Ki Hun Kim (KIST)

Bio 3D printing ink and scaffold containing bone regenerate mineral nanoparticles

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Whitlockite is a calcium phosphate-based ceramic. It contains Mg²⁺ ions, which plays an important role in bone metabolism like bone growth and osteoporosis. As the second most abundant mineral in living bone, Whitlockite occupies 25–35 wt % of the inorganic portion of human bone. We are going to make bone-like bio 3D ink and scaffold using whitlockite and hydroxyapatite and analyze them. That's because 3D printing technology is necessary to output a customized implant to be applied during surgery in-situ. The 3D printing ink and scaffold is composed of whitlockite synthesized by a large-scale precipitation synthesis method and a small amount of polyvinyl alcohol (PVA) was made using an inkjet 3D printer. The bio-ink and scaffold were shown by scanning electron microscopy (SEM), porosity, Thermogravimetric analysis (TGA), and compressive strength testing. These results suggest that whitlockite has excellent potential for application in bone tissue engineering.

Oral Presentation : ANAL2.O-7

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:10

Chair: Ki Hun Kim (KIST)

Simulation of Modified the Morphology of Fe Complex Nanorods Photoanode with Diverse Aspect Ratio for Enhancing the Efficient Oxygen Evolution Reaction

Sohyun Kang, Jaebeom Lee*

Chemistry, Chungnam National University, Korea

The hydrogen production thorough the photoelectrochemical (PEC) water splitting ($2H_2O \rightarrow 2H_2 + O_2$) system is promising system to store solar energy in a clean, low-cost, efficient, and large-scale. Water-splitting technologies depend on a series of electrochemical reactions such as oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) on the electrode surface. The quantity of evolution is able to check the chemical activity of the electrode. However, the reactions have many obstacles to produce oxygen and hydrogen. One of the main problems for the overall efficiency of water splitting is the sluggish kinetics of OER, which involves multiple steps of proton-coupled electron transfer. To defeat the kinetic barrier at a relatively high chemical activity, cost-effective and highly efficient catalysts are required. Herein, the alignments of the Fe complex nanorods along the different magnetic fields are introduced. This nanorods supported on Fluorine-doped tin oxide (FTO) glass facilitates the diffusion of gaseous products (hydrogen and oxygen). Therefore, tuning the electronic structure toward having a chemically active surface area on electrode enhances the chemical activity and outstanding stability for OER in alkaline electrolyte.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:14

Chair: Ki Hun Kim (KIST)

Enhanced electrochemical properties of iodine doped LiFeBO_3 as a cathode for lithium-ion battery

Yujin Jeong, Youngil Lee*

Department of Chemistry, University of Ulsan, Korea

As a cathode material for high-capacity lithium-ion batteries, LiFeBO_3 (LFB) has a higher theoretical capacity of 220 mAh/g than that (170 mAh/g) of LiFePO_4 and is eco-friendly and inexpensive. Due to the disadvantage of poor electrical conductivity, however, various studies have been conducted to improve this characteristic. Herein, we have studied to improve the electrical conductivity by doping iodine having high electronegativity in oxygen sites of LiFeBO_3 . Iodine doped $\text{LiFeBO}_{3-x}\text{I}_{2x}$ has been synthesized by solid-state reaction using planetary ball mill. Solid-state NMR and XRD have been measured to characterize the microstructure and crystal structure of prepared material. Via XRD pattern, it is confirmed that monoclinic single-phase is changed to vonsenite-like phase by iodine doping in LFB. This phase transition to vonsenite can be expected to increase the theoretical capacity. To observe the effect of iodine doping on the electrochemical properties, the electrochemical performances of the synthesized material have been studied by Galvano static charge/discharge test.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:18

Chair: Ki Hun Kim (KIST)

Simple Infrared spectroscopic identification of faulty pre-coated metal products

Woosuk Sohng, Hoeil Chung^{1,*}

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PCM, a pre-coated metal panel used in the manufacture of various home appliances, can be easily processed into the intended form of the target product, making it easier to mass-produce and further improving the appearance of the product. So, the quality of PCM paint during the production process is more important to ensure the high value of PCM-based products. For that reason, defects in PCM substrates are one of the most challenging tasks, and simple analysis methods are required to quickly identify defects in products. In this study, infrared (IR) spectroscopy has been used to identify faulty 1) grey-silver PCMs contained with and without a phosphate epoxy (2.0%), 2) normal and violet colorant-contaminated (0.2%) black PCMs, and 3) normal, violet colorant-contaminated (0.5%), and yellow colorant-contaminated (0.1%) white PCMs samples. A strategy for improving the accuracy of the identification analysis, a temperature-perturbed infrared measurement was incorporated with 2T2D correlation analysis. When 2T2D correlation analysis was conducted using spectra with temperature changes, the identification of the three sample groups were significantly improved over the principal component analysis. According to the 2T2D correlation analysis, the effectiveness of capturing different spectral variation between the normal paint PCM and the defective paint PCM by temperature contributed to the improvement in identification.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:22

Chair: Ki Hun Kim (KIST)

Lipidomic profiling on the effects of particulate matter exposure in mice using LC-MS approach

Seo Young Jang, Dain Kim, Geum-Sook Hwang*

Western Seoul Center, Korea Basic Science Institute, Korea

Particulate matter (PM) is major environmental risk factors in worldwide, and related to human such as respiratory organ, cardiovascular, and nervous system. Recently, many researches have been reported effect by exposure to PM in biological system, whereas the molecular mechanism is not clear. We observed the metabolic changes in response to PM with a diameter 2.5-10um (PM10) exposure in mouse model. In this study, C57BI/6J mice (male) were exposed to PM10 or clean air for 3weeks in champers. We performed global lipid profiling of hippocampus from mice to estimate metabolic alteration using ultra performance liquid chromatography/quadrupole time of flight mass spectroscopy (UPLC/Q TOF MS). We identified 300 lipids in hippocampus. Partial least squares - discriminant analysis (PLS-DA) score plots showed a separation between the PM10 group and control group. We found changes in lipid such as free fatty acid, ceramide, diacylglycerol and phospholipid species in PM10 exposed to mice compared to control. Most of phospholipid species were increased in PM10 exposed mice compared to control, whereas free fatty acid, ceramide and diacylglycerol species were decreased in PM10 exposed group. This study demonstrates that the LC-MS based-lipid profiling can be a used to understand the metabolism of PM10 exposed group on biological system.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:26

Chair: Ki Hun Kim (KIST)

Liquid Chromatography/Mass Spectrometry of Marine Biotoxins with Simultaneous Screening and Identification by Product Ion Spectra

Sanggil Lee, Hyun Joo An^{1,*}

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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 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. Methods were optimized using commercially available reference standards such as gymnodimine-A, 13-desmethyl-spirolide C, pinnatoxin-E, F, G. Mixtures of CIs were separated according to hydrophobicity on C18 column and profiled by accurate molecular weight. Tandem MS (MS/MS) was performed while adjusting CID energy to generate an optimal fragment pattern for identifying CI types. 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 using newly developed analytical platform. This research was supported by a grant (20163MFDS64) from Ministry of Food and Drug Safety in 2021.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:30

Chair: Ki Hun Kim (KIST)

Characterization of hetero-oligomeric cross-talk in Amyloid- β (1-42) using ion mobility mass spectrometry.

Dongjoon Im, MyungKook Son, Chae Ri Park, Sooyeon Chae, Dongvin Kwak, Hugh I.

Kim*

Department of Chemistry, Korea University, Korea

Amyloid- β (1-42) has two additional hydrophobic residues at the C-terminal end compared to amyloid- β (1-40). In our previous study, we reported their fibrillation kinetics and structures at monomer level revealing the two peptides to have similar structural properties in solution phase, yet Amyloid- β (1-42) having focal localization of the radius of gyrates distribution relative to Amyloid- β (1-40). Also taking account that homo-oligomerization was favored in Amyloid- β (1-42), it has been discussed that the two hydrophobic residues to contribute to the acceleration of hydrophobic clustering. Moreover, mixing of these two primary structure-similar peptides formed hetero-oligomers at early aggregation stage resulting in kinetical delay of the fibrillation process. Based on these previous observations, we designed a homologous peptide to delay fibrillation process by disturbing intramolecular hydrophobic interactions between peptides. In order to interrupt the self-assembly of wild type Amyloid- β (1-42) in the same manner, designed mutants should have similar structural properties to wild type at monomer level. Formation of the Amyloid- β (1-42) hetero-oligomer was monitored with ion mobility mass spectrometry. Structural analysis using multiple biophysical approaches, including circular dichroism (CD), solution phase small angle X-ray scattering (solution SAXS), and molecular dynamics (MD) simulation, provided insights into the molecular level mechanism of the cross-talk in Amyloid- β (1-42).

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:34

Chair: Ki Hun Kim (KIST)

Development and Application of Liquid Handler for the Automated Pretreatment of TEMPO-FRIPS

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¹*Department of Chemistry, Sogang University, Korea*

In analytic chemistry, robust and precise pre-treatment is essential for effective chemical reactions. Many commercial liquid handling robots have been developed to meet these needs, like reducing the laborious and time-consuming work. In this research, we devised a liquid handling robot suited for the TEMPO-FRIPS reaction by adopting the hardware of Opentrons OT-1. The parts for the framework, such as aluminum profile, Derlin V-slot wheel, belt, pulleys were purchased online. Some parts were fabricated by CNC machine, and other parts were 3D-printed. The geometry of the frameworks was optimized by trial and error. In the sense of software, the LabVIEW program was utilized to control a microprocessor, Arduino Due electronically. In the plan, we are planning to add vortex mixer, thermostat, centrifuge for the TEMPO-FRIPS reaction. After all functional parts are made, we will apply it to various of TEMPO-FRIPS experiments.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:38

Chair: Ki Hun Kim (KIST)

Modification of Indium Tin Oxide with G6-OH PAMAM Dendrimer-Encapsulated Pt Nanoparticles for the Enhancement of Electrochemiluminescence

Jiwoo Kim, Joohoon Kim*

Department of Chemistry, Kyung Hee University, Korea

In this study, we report surface modification of indium tin oxide (ITO) electrode with a hydroxyl-terminated polyamidoamine (PAMAM) dendrimer-encapsulated Pt Nanoparticles (hydroxyl-terminated Pt DENs) for improved electrochemiluminescence due to catalytic effect of the Pt DENs. Electrochemiluminescence (ECL) is a process in which species generated at electrodes undergo high energy electron transfer reactions to form excited states that emit light. ITO electrodes have features of good optical transmittance and excellent electrical conductivity, and are thus used to image electrochemiluminescence. However, there is limitation in that the electron transfer kinetics of ECL-related reactions at the electrode surface is low. Thus, methods of modifying the surface of the ITO electrode especially with catalytic nanoparticles to improve the kinetics are necessary to be studied. Based on this, it was reported that the ITO electrode could be modified with amine-terminated Pt DENs.¹ By modifying the surface of the ITO electrode with hydroxyl-terminated Pt DENs, we herein expand the types of catalysts, amine-terminated Pt DENs to hydroxyl-terminated Pt DENs, that can be grafted on the surface of ITO electrode for improved ECL.1. S. B. Lee, Y. Ju, Y. Kim et al., Chem. Commun., 2013, 49, 8913-8915

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:42

Chair: Ki Hun Kim (KIST)

Analysis of photothermal effect with different size of Bi-Te Covered Nanorods on 2D monolayer and 3D spheroid neuroblastoma cells

Chae ri Park, MyungKook Son, Dongjoon Im, Sooyeon Chae, Dongvin Kwak, Hugh I.

Kim *

Department of Chemistry, Korea University, Korea

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

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:46

Chair: Ki Hun Kim (KIST)

Nanoparticle Size Determines the Affinity of High-Density Lipoprotein Particles for Pegylated Gold Nanoparticles in Biomolecular Corona Formation

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When nanoparticles come in contact with the biological fluids, some of biomolecules, especially proteins, immediately adsorb on the surfaces of nanoparticles, which leads to protein coronas. It has been known that protein coronas play an important role in the biocompatibility of nanoparticles, and precise understanding of interaction between nanoparticles and biomolecules is critical for nanomaterials safety. In this study, various analysis techniques were utilized in a combined way to understand the properties of protein coronas, which included TEM, nanoparticle tracking analysis, UV-VIS spectrophotometry, and gel electrophoresis. Using the techniques, formation of biomolecular coronas of high-density lipoproteins (HDLs) on the pegylated gold nanoparticles of various sizes (20 – 150 nm diameter) were investigated quantitatively, which revealed an explicit increase in the affinity of HDLs for less-curved nanoparticle surfaces, further suggesting that the adsorption is initially governed by the particle nature of HDLs rather than its constituent biomolecules such as apolipoproteins.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:50

Chair: Ki Hun Kim (KIST)

Investigation of Mechanisms and Drug Uptake in Human neuroblastoma SK-N-SH Cells in 3D Spheroids

Sooyeon Chae, Dongvin Kwak, Hugh I. Kim*

Department of Chemistry, Korea University, Korea

Neuroblastoma is an uncommon pediatric cancer and to be diagnosed in the first year of life. It is a complex and heterogeneous disease therefore many factors, such as age, gene mutation, cell differentiation level, and stage of disease, affect therapeutic diagnose. As neuroblastoma belongs to heterogeneous disease, cancer cells can show distinct morphological and phenotypic profiles including cellular morphology, gene expression, metabolism, motility, proliferation, and metastatic potential. To maximize treatment efficiency, tailor treatment is applied to each patient. However, it is still challenging because of complexity of disease and the different response between 2-dimensional (2D) model system and real tumor. 3D spheroids of tumor cells can reflect the characteristics of solid tumors by retaining cell-cell interactions and microenvironments such as hypoxic conditions that better reflect drug resistance than 2D models. This model system can provide more comprehensive information about the preclinical drug response of neuroblastoma cells inside the solid tumor. Several studies approach to explore the differences in 3D spheroids and 2D cells. However, it is still challenging to understand differences in morphology and microenvironments in 3D spheroids compared to those in 2D monolayers that influence the drug response and the mechanisms of action. In this study, we investigated the pathology mechanisms and drug uptake in SK-N-SH neuroblastoma cells cultured in 3D spheroids compared to those in 2D monolayers using electrospray ionization mass spectrometry (ESI-MS) and computational fluid dynamics.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:54

Chair: Ki Hun Kim (KIST)

Structural elucidation of glycoconjugates in humanized mouse liver tissue using LC-MS/MS

Dongtan Yin, Hyun Joo An^{1,*}

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

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

Mouse is the most common model in the preclinical test and liver tissue is used to test the drug metabolism and prediction of in-vivo kinetics. Drug metabolism is an important issue in preclinical test for produce more safe and effective candidates. However, the general success rate of new drug candidates during clinical trials is still low. One outstanding explanation is difference of glycosylation, in which inter-species differences between the mouse models and humans. Recent studies have shown that two critical differences (Neu5Gc, alpha-gal) have been identified between humans and other mammals. Especially, Neu5Gc epitopes could lead to several inflammatory disorders. Also, alpha-gal is known to cause of severe hypersensitivity reactions after xenotransplantation. For this reason, "humanized" mouse models such as triple-knockout (CMAH/GGTA1/iGb3S) models related to Neu5Gc and alpha-gal epitopes have been developed. However, there is still lack of the study on qualitative and quantitative glycoconjugates structure details. Here, we elucidated the structure of glycan and glycolipids obtained from mouse liver tissue by LC-MS/MS in both negative and positive ion detection mode. Negative ion mode MS/MS provides sensitive detection sialic acid-containing structures with lower background noise whereas positive mode MS/MS produces more detailed lipids fragment ions such as ceramide. The analysis data demonstrated the presence of known Neu5Gc and alpha-gal antigens. Furthermore, we could identify differently glycosylation, between humans and mouse such as sialylated HexNAc, unique Neu5Ac-containing N-glycan, co-existence of NeuAc and NeuGc containing N-glycan. Finally, this structure information provides a reference to other new potentially functional glycan structures.

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

Oral Presentation of Young Analytical Chemists II

Room 301 (Live Streaming) THU 11:57

Chair: Ki Hun Kim (KIST)

Real-time Monitoring Growth of Single Bacteria using Droplet-based Microfluidics and Identification of Bacterial Gas Metabolism in Microenvironment

Sunghyun Ki, Dong-Ku Kang^{1,*}

Chemistry, Incheon National University, Korea

¹*Department of Chemistry, Incheon National University, Korea*

Droplet-based microfluidics (DMF) has been developed in analytical chemistry to analysis chemical and biological components such as viruses, bacteria and nucleic acid. Generation of monodisperse droplets is important for the accurate and sensitive analysis where droplets must be kept in stable for various applications including single-molecule detection and droplet digital PCR. To guarantee stability of droplets, droplets are normally generated with oil and surfactant. Among various surfactants, PFPE-PEG-PFPE surfactant demonstrated have been widely used in DMF that surfactant was introduced from Weitz group because of stability and biocompatibility. However, there are no studies on gas crosstalk between droplets. Therefore, we experimentally confirmed that gas crosstalk occurred between droplets. *E. coli* K-12 cells were encapsulated within droplets for the cultivation, and gas crosstalk was identified with neighboring droplets that contain the phenol red. Since bacteria produce ammonia gas during cultivation, penetration of ammonia gas initiates a color change of phenol red-containing droplets. Ammonia gas was artificially produced through a chemical reaction between ammonium chloride and sodium hydroxide within droplets to experimentally confirmed that the ammonia gas can transport into neighboring droplets. We also confirmed that surfactant density affects the gas permeability between droplets. In this study, it was verified that crosstalk of ammonia gas, a bacterial metabolite, was occurred between droplets encapsulated by PFPE-PEG-PFPE surfactants. Our results suggest that DMF can be used for monitoring of living bacteria by bacterial metabolites and this phenomenon can be applied for microenvironmental chemical reaction that required gas as catalysts.

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

Oral Presentations by Young Life Chemists

Room 305 (Live Streaming) THU 10:00

Chair: Hak Joong Kim (Korea University)

pH-dependent regulation of p62/SQSTM1 during autophagy

Hyun Kyu Song

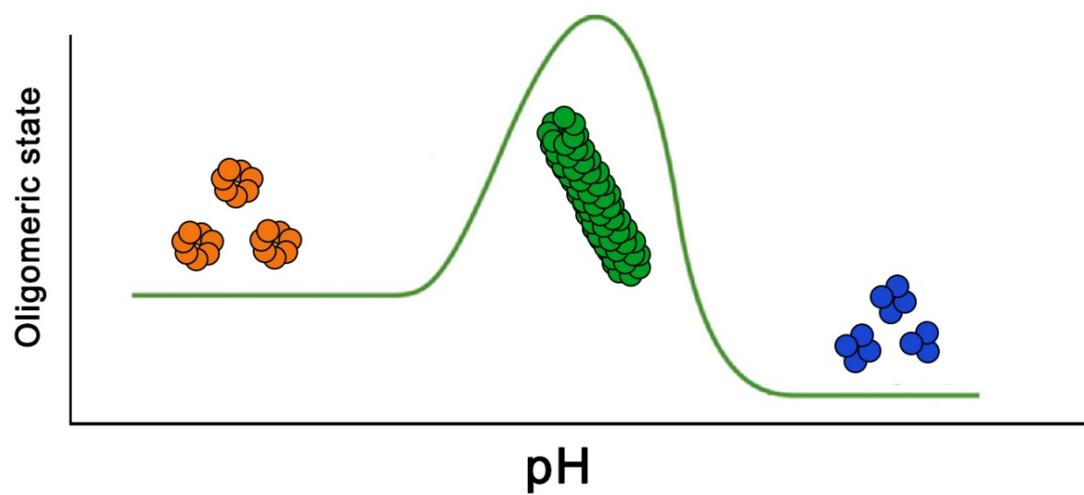
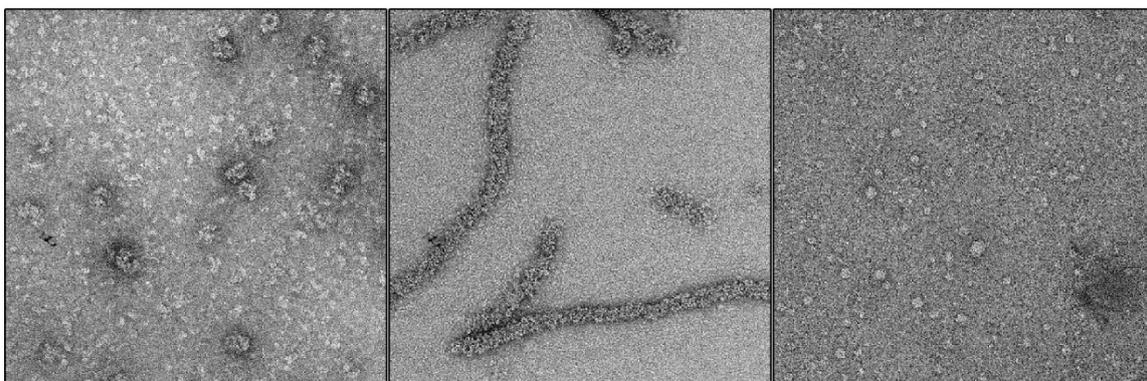
Division of Life Sciences, Korea University, Korea

During macroautophagy/autophagy, p62/SQSTM1 autophagy adaptor plays dual roles as a key mediator of cargo selection and as an autophagic substrate. The p62 links N-degrons and/or ubiquitinated cargoes to the autophagosome by forming homo- or hetero-oligomers, although its N-degron recognition and oligomerization mechanisms are not well characterized. My laboratory found that p62 is a novel type of N-recognin whose ZZ domain provides a negatively-charged binding pocket for Arg-charged N-degron (Nt-Arg), a prototype type-1 substrate. Although differences in binding affinity exist for each N-degron, p62 also interacts with type-2 N-degrons, such as Nt-Tyr and Nt-Trp. Intriguingly, interactions between p62's ZZ domain and various N-degrons are greatly influenced by pH-dependent p62 oligomerization via its PB1 domain. Because cellular pH conditions vary from neutral to acidic depending on the stage of autophagy, the pH-dependent regulation of p62's oligomerization must be tightly coupled with the autophagic process.

pH 7.5

pH 6.0

pH 4.5



GREEN CHEMICAL SOCIETY

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

Oral Presentations by Young Life Chemists

Room 305 (Live Streaming) THU 09:00

Chair: Kwon-Yul Ryu (University of Seoul)

DEVELOPING A QUANTITATIVE DETECTION METHOD FOR P53 PROTEIN PHOSPHORYLATION USING CAPILLARY ELECTROPHORESIS

Min-Jung Kang^{*}, Eda Ates¹

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Science and Technology, Korea*

Post transcriptionally modified, tumor suppressor p53 protein plays a critical role in the regulation of genes that control cell cycle arrest, apoptosis and senescence. Therefore, finding a quantitative analyses of post-translational modifications are useful for predicting PTMs, biomarker discovery and understanding the relationship between protein modification and cancer development. In our study, we have developed a sensitive, reproducible, cost effective and quantitative capillary electrophoresis-laser-induced fluorescence (CE-LIF) method for the analysis of phosphorylated peptides of p53. The synthetic substrate and its 4 phosphorylated products were used to validate the capability of the method. The substrate Pep1, which reached the detection window after 2.00 ± 0.02 min, and followed by the phosphorylation products Pep2, Pep3, Pep4, and Pep5, which migrated slower. The LOD and LOQ were obtained as follows; 0.3 and 1 ng/mL for Pep1, 8 and 29 ng/mL for Pep2, 10 and 28 ng/mL Pep3, 2 and 7.8 ng/mL for Pep4, finally 0.7 and 2.5 ng/mL for Pep5. The application of method to cancer cell line showed that different phosphorylation on Ser 6, Ser 9, Ser15 and Ser20 reproducibility. The reproducibility was within 9.2 %. Because of its low limit of detection and accurate quantitative analysis ability, it has the potential for high throughput screening of phosphorylated p53 protein for discovery of therapeutic target and drug program.

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

Oral Presentations by Young Life Chemists

Room 305 (Live Streaming) THU 09:10

Chair: Kwon-Yul Ryu (University of Seoul)

Structural and biochemical insights reveal phospholipid transfer activity of PTPIP51 at Endoplasmic Reticulum-Mitochondria Contact sites

Tae Hyun Park, Byung il Lee*

Division of Precision Medicine, National Cancer Center, Korea

In eukaryotic cells, mitochondria are closely tethered to the endoplasmic reticulum (ER) at sites called mitochondria-associated ER membranes (MAMs). Ca²⁺ ion and phospholipid transfer occurs at MAMs to support diverse cellular functions. Unlike those in yeast, the protein complexes involved in phospholipid transfer at MAMs in humans have not been identified. Here, we determined the crystal structure of the tetratricopeptide repeat domain of PTPIP51 (PTPIP51_TPR), a mitochondrial protein that interacts with the ER-anchored VAPB protein at MAMs. The structure of PTPIP51_TPR showed an archetypal TPR fold, and an electron density map corresponding to an unidentified lipid-like molecule probably derived from the protein expression host was found in the structure. We revealed functions of PTPIP51 in phospholipid binding/transfer, particularly of phosphatidic acid, in vitro. Depletion of PTPIP51 in cells reduced the mitochondrial cardiolipin level. Additionally, we confirmed that the PTPIP51-VAPB interaction is mediated by the FFAT-like motif of PTPIP51 and the MSP domain of VAPB. Our findings suggest that PTPIP51 is a phospholipid transfer protein with a MAM-tethering function similar to the ERMES complex in yeast.

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

Oral Presentations by Young Life Chemists

Room 305 (Live Streaming) THU 09:20

Chair: Kwon-Yul Ryu (University of Seoul)

Raman-active and clickable APEX probes for proximity-dependent proteomic labeling in living cell

Mohamed Elgawish

Chemistry, Korea University, Egypt

APEX-proximity labeling (PL)-based technique has emerged in recent years as a powerful tool for catching stable and transient protein interactions on a minute scale in different subcellular compartments and whole organisms. When the substrate, biotin-phenol, is added, the APEX enzyme is activated by rapid treatment with H₂O₂ to create highly reactive phenoxyl radicals that form a covalent bond within a 20 nm labeling radius with protein residues of electron-rich amino acids. Even with the broad application of biotin-phenol as APEX substrate, there may be concerns over the cellular impact of biotin-phenol. Novel APEX substrate for vibrational spectroscopy and confocal fluorescence microscopy are presented here. A panel of alkyne-containing aromatic compounds was synthesized and screened their activity towards APEX. 4-((4-ethynylphenyl)buta-1,3-diyne-1-yl) phenol (4-EPBDP) was defined in different subcellular compartments, including nucleus, the endoplasmic reticulum, and mitochondria, as a novel probe with significantly greater protein reactivity. 4-EPBDP possesses a unique feature, a conjugated structure connecting two internal alkynes, two phenyl groups, and one terminal alkyne for a strong Raman scattering signal. The terminal alkyne function as a clickable tag for fluorescence microscopy or mass spectrometry for proteomic profiling. We found from confocal fluorescence microscopy that 4-EPBDP allows rapid labeling with surprisingly high specificity and low cell toxicity compared to biotin-phenol. Besides, the 4-EPBDP probe demonstrated vibrational solvatochromism, making it a promising molecule by measuring the alkyne peak frequency change at 2200 cm⁻¹ in the cell-free window to detect the local environment of specific subcellular compartments. Therefore, we have introduced a new proximity labeling application for Raman spectroscopy to test a variety of subcellular environments. In summary, we develop PL probes with high labeling selectivity, allowing for the first time, the proximity-dependent proteins labeling in various subcellular compartments using Raman microscopy.

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

Oral Presentations by Young Life Chemists

Room 305 (Live Streaming) THU 09:30

Chair: Kwon-Yul Ryu (University of Seoul)

Studies of apoptosis inducing small molecule and synthetic ion transporters

Sang-Hyun Park, Injae Shin*

Department of Chemistry, Yonsei University, Korea

Apoptosis, or programmed cell death, is a fundamental biological process which is involved in normal development, regulation of the immune system, development of the nervous system, and tissue homeostasis. Unwanted or damaged cells are eliminated by the apoptotic process. There are number of ways to regulate the apoptosis process by using small molecules or synthetic ion transporters. In various cancer cells, heat shock protein 70 (Hsp70) is overexpressed in lysosomes and functions as a lysosome stabilizer through association with lysosomal membranes. Here we describe a small molecule named as apoptozole (Az) that translocates into lysosomes to induce lysosomal membrane permeabilization (LMP) and promotes lysosome-mediated apoptosis. Furthermore, cellular ion concentrations are tightly regulated by the action of a variety of ion transporters and channels. Perturbations in the intracellular concentrations of ions such as chloride, calcium and potassium ions are closely correlated with the onset of apoptosis. To date, several transporters capable of promoting apoptosis have been reported for example, diamide-strapped calix[4]pyrrole-1 (DSC4P-1) or squaramide-3 (SA-3) by disrupting intracellular ion homeostasis. Here we have elucidated the mechanism of synthetic ion transporters (DSC4P-1, SA-3, and 8FC4P). The synthetic ion transporters increase intracellular Cl⁻ and Na⁺ concentrations to induce osmotic stress in cells and leads to caspase-dependent apoptosis. Such findings inform that heat shock protein 70 or intracellular ions can be set as targets to develop anticancer agents that have apoptosis as mode of action.

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

Oral Presentations by Young Life Chemists

Room 305 (Live Streaming) THU 09:40

Chair: Kwon-Yul Ryu (University of Seoul)

Single-molecule observation of the directionality of bacteriophage DNA ejection

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¹*Department of Chemistry, Sogang University, Korea*

The bacteriophage DNA ejection is a vital process for viral life. Therefore, there have been lots of studies done for bacteriophage DNA ejection. Since bacteriophage λ has been a model for the virus for many decades, there have been many studies to determine the directionality of the phage λ DNA ejection. However, the directionality of bacteriophage DNA ejection remains unclear. Given these concerns, this research offers novel approaches to the phage λ DNA ejection's directionality by visualizing sequence-specific stained single DNA molecules. Our previous studies provide an effective method to analyze λ DNA directionality by observing A/T-specific patterns of λ DNA [1, 2]. We treated λ phage DNA with glutaraldehyde, stained ejected DNA with A/T-specific reagents to visualize a viral capsid, and tethered DNA. Also, we used several dyes such as Silicone-Rhodamine polypyrrole and a combination of netropsin and YOYO-1 to perform sequence-specific staining for observation of pattern on λ DNA ejected from λ phages and commercial λ DNA for comparison. Finally, we did a quantitative analysis of λ phage DNA ejection to reveal DNA ejection's directionality. The directionality of phage DNA ejection is one of bacteriophages' essential characteristics; therefore, this study provides new approaches to reveal phage physiology.

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

Oral Presentations by Young Life Chemists

Room 305 (Live Streaming) THU 09:50

Chair: Kwon-Yul Ryu (University of Seoul)

The antipsychotic drug Clozapine suppresses degradation of RGS4 via the Arg/N-degron pathway.

Taerim Oh, Min Jae Lee^{1,*}

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Korea*

¹*College of Medicine, Biochemistry, Seoul National University, Korea*

Although diverse antipsychotic drugs have been developed for the treatment of schizophrenia, most of their mechanisms of action remain elusive. Regulator of G-protein signaling 4 (RGS4) has been reported to be linked, both genetically and functionally, with schizophrenia and is a physiological substrate of the arginylation branch of the N-degron pathway (Arg/N-degron pathway). Here, we show that the atypical antipsychotic drug clozapine significantly inhibits proteasomal degradation of RGS4 proteins without affecting their transcriptional expression. In addition, the levels of Arg- and Phe-GFP (artificial substrates of the Arg/N-degron pathway) were significantly elevated by clozapine treatment. In silico computational analysis model suggested that clozapine may interact with active sites of N-recogin E3 ubiquitin ligases. Accordingly, treatment with clozapine resulted in reduced polyubiquitylation of RGS4 and Arg-GFP in the test tube and in cultured cells. Clozapine attenuated the activation of downstream effectors of G protein-coupled receptor signaling, such as MEK1 and ERK1, in HEK293 and SH-SY5Y cells. Furthermore, intraperitoneal injection of clozapine into rats significantly stabilized the endogenous RGS4 protein in the prefrontal cortex. Overall, these results reveal an additional therapeutic mechanism of action of clozapine: this drug post-translationally inhibits the degradation of Arg/N-degron substrates, including RGS4. These findings imply that modulation of protein post-translational modifications, in particular the Arg/N-degron pathway, may be a novel molecular therapeutic strategy against schizophrenia.

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

Oral Presentations for Young Scholars in Organic Division

Room 304 (Live Streaming) THU 15:30

Chair: Eunha Kim (Ajou University)

Oxidatively-induced reductive elimination in transition metal-catalyzed C–H functionalizations

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

¹*Korea Advanced Institute of Science and Technology, Korea*

²*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

³*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Since the 1970s, significant advances in transition metal-catalyzed coupling processes have provided a range of synthetic platforms for synthetic and industrial chemistry, based on the distinct reactivities complementary to the conventional organic transformations, thereby instigating detailed exploration on the mechanistic details of the catalytic cycle. Among the mechanistic constituents, in particular, reductive elimination (RE) process has been extensively studied as it comprises a key step where the desired chemical bond is constructed. Seminal studies revealed that the oxidation of post-transmetalation intermediate often significantly facilitates the RE process by reducing the energy barrier for the bond formation. Although this process, oxidatively-induced reductive elimination (ORE), has been sporadically reported for a range of organometallic systems, its deliberate utilization on catalytic procedures has been still underexplored. The current series of studies deals with the high-valent pathway in C–H aryl- and methylation via oxidative coupling process, using Cp*Ir(III), Cp*Rh(III), and (p-cymene)Ru(II) catalyst systems with a range of oxidation systems. After verifying that the ORE mechanism is commonly operative in the C–C bond formation with those catalyst systems, its applications on the development of novel synthetic methodology are introduced. Furthermore, in addition to the chemical oxidants, photocatalytic redox cycle and even the transient oxidation via metal-to-ligand charge transfer were also shown to generate the key high-valent intermediate, eventually leading to the C–C bond-forming reductive elimination under catalytic conditions.

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

Oral Presentations for Young Scholars in Organic Division

Room 304 (Live Streaming) THU 15:45

Chair: Eunha Kim (Ajou University)

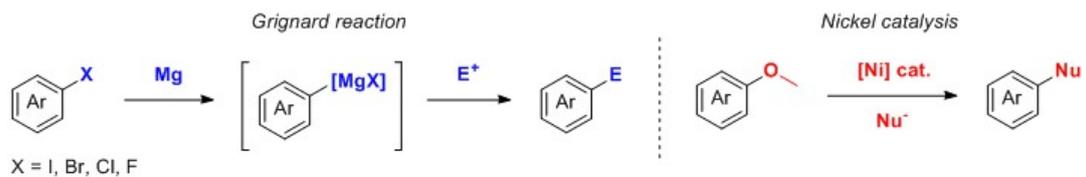
Preparation of Grignard Reagents by C-O Bond Activation

Ewa Pietrasiak^{*}, Eunsung Lee^{*}

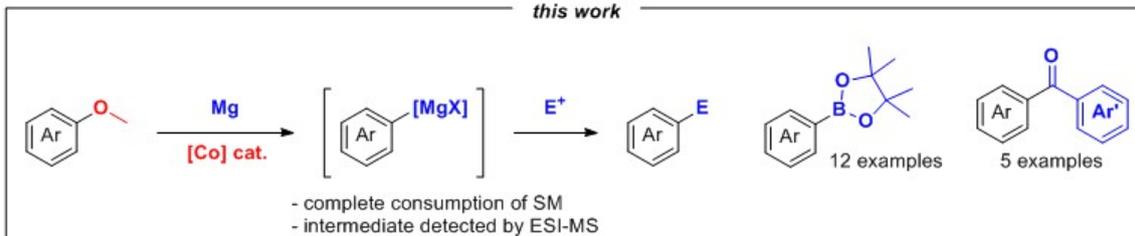
Department of Chemistry, Pohang University of Science and Technology, Korea

Organomagnesium reagents (Grignard reagents) belong to the most common organometallic reagents applied in organic synthesis.[1] Typically, Grignard reagents are prepared from alkyl/aryl halides (iodides, bromides, chlorides or even fluorides) in a reaction with magnesium metal proceeding via two subsequent electron transfer steps.[2] In contrast, C-O bonds are typically inert towards magnesium and examples of Grignard reagent formation from ethers proceeds well only in case of allyl substrates.[3] Consequently, transition metal catalysts (notably nickel complexes) are usually used to cleave C-O bonds.[4] Herein, we demonstrate that this transformation can be activated in the presence of a cobalt catalyst, previously applied by our group for C-F bond activation.[5,6] The resulting organocobalt intermediate undergoes transmetalation to magnesium effectively providing a Grignard reagent derived from the ether. The presence of this intermediate was indirectly confirmed by reactivity tests and directly by mass spectroscopic analysis. In the presence of pinacol borane, a series of aromatic and aliphatic ethers could be converted to the corresponding boronic acid esters. A reaction with aldehydes promoted by cerium chloride provided aromatic ketones. These transformations demonstrate the utility of our system in the context of organic synthesis.1. Organometallics 2009, 28, 1598.2. J. Phys. Org. Chem. 2006, 19, 847.3. J. Organomet. Chem. 1969, 18, 249.4. J. Am. Chem. Soc. 2017, 139, 10347.5. Org. Lett. 2018, 20, 7249.6. Org. Lett. 2020, DOI 10.1021/acs.orglett.0c02752.

previous work



this work



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

Oral Presentations for Young Scholars in Organic Division

Room 304 (Live Streaming) THU 16:00

Chair: Eunha Kim (Ajou University)

Breaking Symmetry in Well-Organized Self-Assembly by Single Atom Mutation on Critical Residue

Byung-Chang Oh, Eunyoung Yoon¹, Jintaek Gong, Jaewook Kim, Russell W. Driver², Wooyoung Kim³, Hee-Seung Lee*

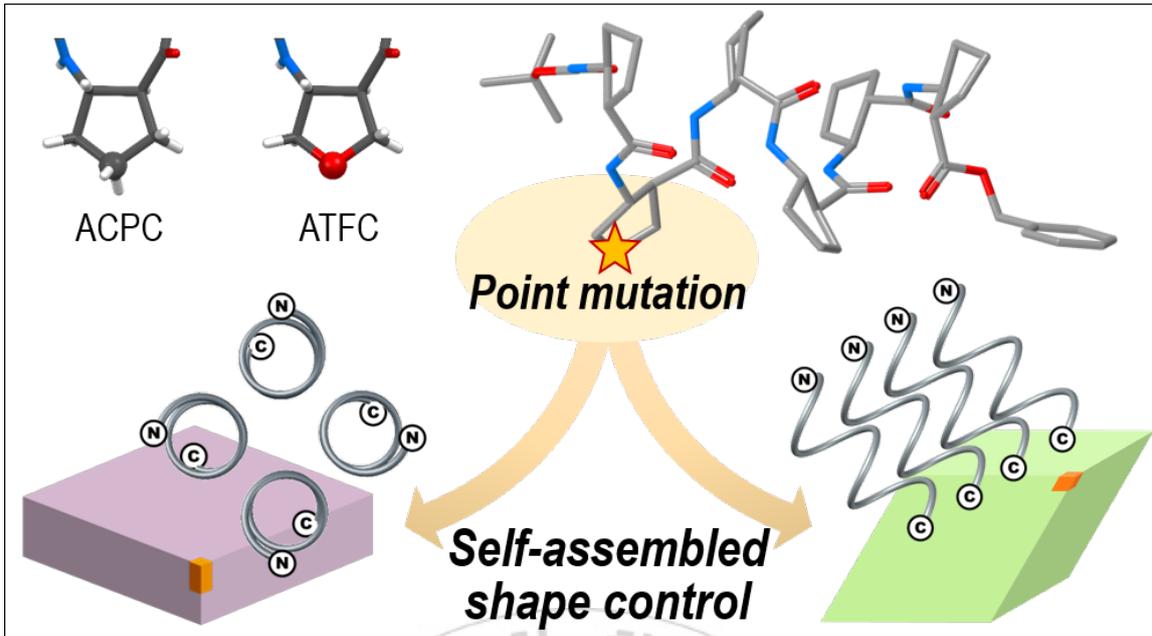
Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

¹*Korea Research Institute of Chemical Technology, Korea*

²*Department of Chemistry and Physics, Nova Southeastern University, United States*

³*Department of Chemistry, KAIST, Korea*

Generation of well-defined 3D self-assembled structures from exclusively unnatural peptides is drawing considerable attention at present. However, achieving the desired molecular orientation and alignment within a fixed supramolecular structure is formidable, because the underpinning principle governing the self-assembly process is not yet understood thoroughly. We addressed this challenge by conducting systematic studies on self-assemblies and persistent solid-state structural analysis using congener short β -peptide foldamers, to find a molecular condition that changes the symmetry during their self-assembly. A scanning monomer for subtle electronic perturbations on hydrophobic foldamers induced a previously inaccessible solid-state geometric split in a sequence specific manner. This enabled us to identify the most susceptible site for foldamer association, generating disparate self-assembled structures without altering the foldamer length and helix type. This systematic approach will not only provide inspiration for studying conformational polymorphism during self-assembly but will also guide in designing building blocks from scratch to create well-organized assembled architectures with desired shapes.



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

Oral Presentations for Young Scholars in Organic Division

Room 304 (Live Streaming) THU 16:15

Chair: Eunha Kim (Ajou University)

Fluorescent probes for organelle imaging and proteomics

Dhiraj Murale

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

Researchers are extensively trying to achieve comprehensive protein lists for the sub-cellular regions by using mass spectrometry. Organellar-based proteomics has emerged out to be the most rapidly advancing methods to obtain the protein list and functional analysis of those subcellular proteins. Here, we report the rational designs of the BODIPY fluorophores and its second-generation probes for the imaging of subcellular organelle. We envisioned to target the specific organelle by simple modifications of bodipy fluorophore with pyridinium salt, morpholino, alterations for mitochondria, lysosome respectively. In recent times researchers are extensively using Photo-affinity labeling (PAL) strategy in chemical proteomics to study Protein-protein interactions (PPIs).¹ In order to obtain the detailed insights into subcellular proteome by using PAL we have incorporated the photocrosslinking moieties onto the bodipy probes called photocrosslinking bodipy (pcBD). The main success for this pcBD design is, this works better than benzophenone also it has BODIPY fluorophore so can be used as fluorescent tag. Also we proved the utility of photo-crosslinking fluorophore for spatiotemporal protein labeling in complex mixture.² Here we utilized combination of the organelle specific probes and the LC-MS based proteome technology for identification of subcellular proteome.

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

Oral Presentations for Young Scholars in Organic Division

Room 304 (Live Streaming) THU 16:30

Chair: Eunha Kim (Ajou University)

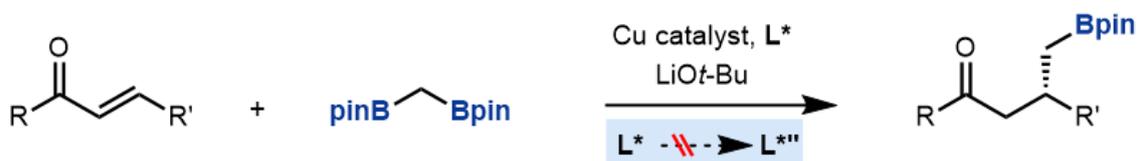
Restoration of catalytic activity by the preservation of ligand structure: Cu-catalysed asymmetric conjugate addition with 1,1-diborylmethane

Byeongdo Roh, Hong Geun Lee*

Department of Chemistry, Seoul National University, Korea

Described herein is a novel reaction engineering protocol to enhance the efficiency of a transition metal catalysed process by strategically preventing ligand degradation. Based on spectroscopic investigations, a decomposition pathway of a chiral phosphoramidite ligand during a Cu-catalysed reaction was identified. The involvement of the destructive process could be minimized under the modified reaction conditions that control the amount of nucleophilic alkoxide base, which is the origin of ligand decomposition. Overall, the strategy has been successfully applied to a new class of asymmetric conjugate addition reactions with bis[(pinacolato)boryl]methane, in which α,β -unsaturated enones are utilised as substrates

"strategic prevention of ligand degradation"



L*: active chiral ligand
L**: inactive chiral ligand

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

Oral Presentations for Young Scholars in Organic Division

Room 304 (Live Streaming) THU 16:45

Chair: Eunha Kim (Ajou University)

Stereodivergent Total Syntheses of Antirhine Alkaloids

Eunjoon Park, Cheol-Hong Cheon*

Department of Chemistry, Korea University, Korea

Antirhine family comprises a small group of the monoterpene alkaloids bearing the indoloquinolizidine scaffold. They possess unique structural features; two-carbon unit connected to the side-chain at the C-20 position rather than at the C-16 position. In addition, they possess thermodynamically less stable anti-relationship between the C-3 and C-15 stereocenters. Moreover, as all C-20 epimers of these natural products are found in nature, which imparts additional structural diversity to this family. Due to the unique structural features of the antirhine family, it is therefore of great interest to develop a general synthetic route to access these family over a long time. Most previous methods to access the antirhine family commenced with a specific starting material containing the key fragment with right stereochemistry at the C-15 and C-20 positions. Subsequent construction of the C/D rings with tryptamine afforded the antirhines. However, these conventional approaches have several limitations. 1) the lack of generality applicable for both antirhine and its congeners, 2) relatively lengthy synthetic sequences to control the C-15 and C-20 stereochemistry, and 3) difficulty in control of the trans relationship between C-3 and C-15 centers. In this presentation, a general synthetic strategy for antirhine alkaloids will be presented. The cyanide-catalyzed imino-Stetter reaction afforded the corresponding indole-3-acetic acid derivative. Subsequent formation of the 6-membered C-ring followed by trans-selective installation of the two-carbon unit at the C-15 position provided a rapid access to the key intermediate. Stereoselective installation of substituents at the C-20 position completed the total syntheses of antirhine, 18,19-dihydroantirhine and their 20-epimers.

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

Oral Presentations for Young Scholars in Organic Division

Room 304 (Live Streaming) THU 17:00

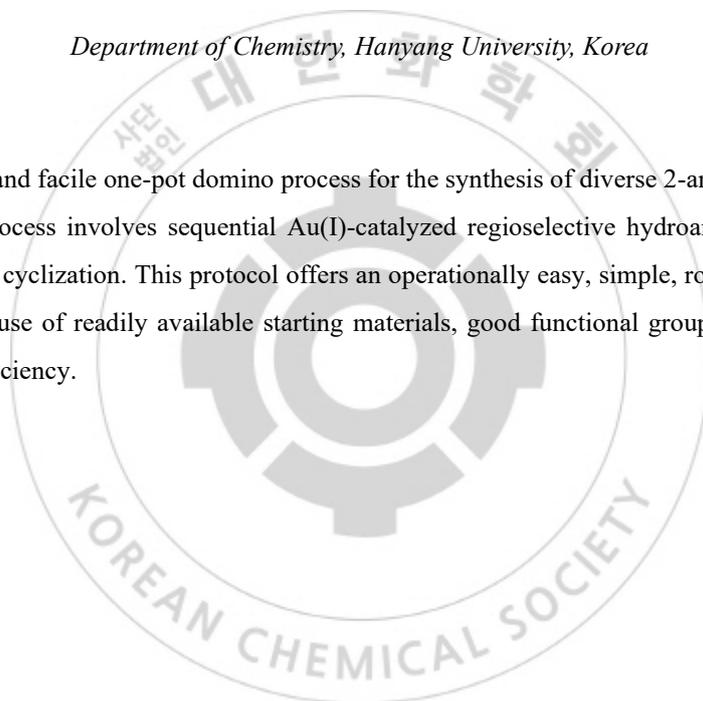
Chair: Eunha Kim (Ajou University)

One-Pot Domino Process for the Synthesis of 2-Aminoindoles

Youngho Kim, So Won Youn*

Department of Chemistry, Hanyang University, Korea

A highly effective and facile one-pot domino process for the synthesis of diverse 2-aminoindoles has been developed. This process involves sequential Au(I)-catalyzed regioselective hydroamination and CuCl₂-mediated oxidative cyclization. This protocol offers an operationally easy, simple, robust, and sustainable approach with the use of readily available starting materials, good functional group tolerance, and high practicality and efficiency.



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

Oral Presentations for Young Scholars in Organic Division

Room 304 (Live Streaming) THU 17:15

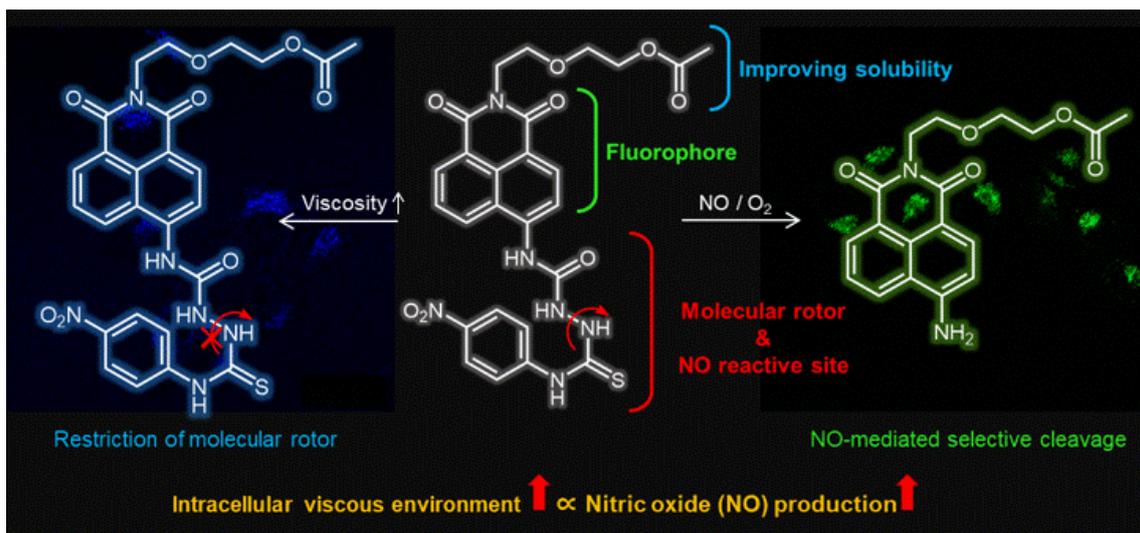
Chair: Eunha Kim (Ajou University)

Naphthalimide-4-(4-nitrophenyl)thiosemicarbazide: A Fluorescent Probe for Simultaneous Monitoring of Viscosity and Nitric Oxide in Living Cells

Sun Young Park, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Intracellular viscosity is a physicochemical factor that determines the outcomes of various biological processes, while nitric oxide (NO) is an essential signaling molecule that controls many cellular processes, including oxidative stress. Anticipating that both may be interrelated with a variety of pathologies, their simultaneous measurement would be highly valuable for the investigation of the pathological condition of cells. However, the development of a sensor for such simultaneous detection has not been attempted yet. Herein, we present the synthesis of naphthalimide-4-(4-nitrophenyl)thiosemicarbazide, probe **1**, and its application to living cells under conditions of lipopolysaccharide or nystatin treatment, adopted as oxidative stress and altered intracellular viscosity models, respectively. The probe showed increased fluorescence in response to elevation of viscosity and NO levels at 470 and 550 nm, respectively, in the solution studies. When the probe was used for a confocal microscopic study of HeLa cells under stressed conditions, simultaneous monitoring of viscosity and NO level elevations was possible through fluorescence imaging using band-pass filters of 420–475 and 505–600 nm, respectively, upon excitation at a wavelength of 405 nm. Interestingly, both the cellular viscosity and NO levels increased together under lipopolysaccharide or nystatin treatment. Therefore, we suggest that probe **1** is a fluorescent chemical probe that enables the monitoring of alterations in intracellular viscosity and NO levels in living cells, which would be valuable in studies of various cellular damage models.



Oral Presentation : **MEDIO-1**

Oral Presentation of Young Medicinal Chemists

Room 306 (Live Streaming) THU 09:00

Chair: Sang Min Lim (KIST)

MeBib Suppressed Methamphetamine Self-Administration Response via Inhibition of BDNF/ERK/CREB Signal Pathway in the Hippocampus

Sonam Jha, Young Ho Seo^{1,*}

College of pharmacy, Keimyung University, Korea

¹*College of Pharmacy, Keimyung University, Korea*

Methamphetamine (MA) is one of the most commonly abused drugs in the world by illegal drug users. Addiction to MA is a serious public health problem and effective therapies do not exist to date. It has also been reported that behavior induced by psychostimulants such as MA is related to histone deacetylase (HDAC). MeBib is an HDAC6 inhibitor derived from a benzimidazole scaffold. Many benzimidazole-containing compounds exhibit a wide range of pharmacological activity. In this study, we investigated whether HDAC6 inhibitor MeBib modulates the behavioral response in MA self-administered rats. Our results demonstrated that the number of active lever presses in MA self-administered rats was reduced by pretreatment with MeBib. In the hippocampus of rats, we also found MA administration promotes GluN2B, an NMDA receptor subunit, expression, which results in sequential activation of ERK/CREB/BDNF pathway, however, MeBib abrogated it. Collectively, we suggest that MeBib prevents the MA seeking response induced by MA administration and therefore, represents a potent candidate as an MA addiction inhibitor.

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

Oral Presentation of Young Medicinal Chemists

Room 306 (Live Streaming) THU 09:10

Chair: Sang Min Lim (KIST)

Macrocyclic Phosphopeptide targeting the Polo Box Domain of Polo-Like Kinase 1

Seong Shick Ryu, Taebo Sim^{1,*}

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

¹*Severance Biomedical Science, Yonsei University, Korea*

Polo-like kinase 1 (Plk1), a serine/threonine kinase, regulates pivotal stages of mitosis including mitotic entry, spindle assembly, centrosome maturation, chromosome segregation and cytokinesis. Commensurate with its critical role in promoting cell proliferation, Plk1 is overexpressed in a broad range of human cancers. Plk1 possesses a conserved N-terminal kinase domain and a non-catalytic C-terminal domain consisting of two tandem polo box motifs that together constitute a phosphopeptide binding Polo Box Domain (PBD). The Plk1-PBD functions as a high affinity phospho-Ser/Thr-binding module. In addition to its substrate targeting and subcellular localization activities, the PBD also regulates Plk1 kinase activity via a mutually auto-inhibitory interaction between the kinase domain and the PBD. Recent studies examining the cellular consequences of targeted disruption of PBD function have demonstrated it to be an attractive target for anti-cancer drug discovery. We synthesized macrocyclic phosphopeptides, which inhibit Plk1-PBD with selectivity among the Plk families. Intracellular anti Plk1-PBD activity was identified by Plk1 delocalization and mitotic failure in HeLa cells. Moreover, we envision that our X-ray co crystal structure will be served as useful guidelines in establishing strategies to rational design of Plk1-PBD targeting agents.

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

Oral Presentation of Young Medicinal Chemists

Room 306 (Live Streaming) THU 09:20

Chair: Sang Min Lim (KIST)

Targeting of EGFR ex20ins mutations for the treatment of NSCLC

Yujin Lee, Kwangho Lee^{1,*}

Medicinal Chemistry and Pharmacology, University of Science & Technology, Korea

¹*Korea Research Institute of Chemical Technology, Korea*

The epidermal growth factor receptor (EGFR) is a tyrosine kinase receptor. It is widely expressed in many cancers, especially non-small cell lung cancer (NSCLC). Mutations such as deletion in exon 19 (del19), L858R in exon 21 and various minor mutations cause the over-expression of EGFR in NSCLC. Erlotinib (Tarceva) & Gefitinib (Iressa) are the 1st generation of EGFR kinase inhibitors for EGFR L858R and del19 mutations. However, their clinical use is ultimately limited due to the mechanism-based toxicity and development of drug-resistance caused by EGFR T790M mutation. Osimertinib (Tagrisso), an irreversible inhibitor, has been approved recently for the 3rd generation treatment option to overcome the short-comings of the first class drug use. However, there are still not enough medical options for various minor mutations such as EGFR G719X, S768I, L861Q and exon 20 insertion (Ex20ins). EGFR G719X, S768I and L861Q mutations are partially responding to current approved tyrosine kinase inhibitors (TKIs), whereas Ex20ins mutations are not responding. In this presentation, new medicinal chemistry strategy will be discussed to address the currently unmet-medical needs for EGFR ex20ins mutations.

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

Oral Presentation of Young Medicinal Chemists

Room 306 (Live Streaming) THU 09:30

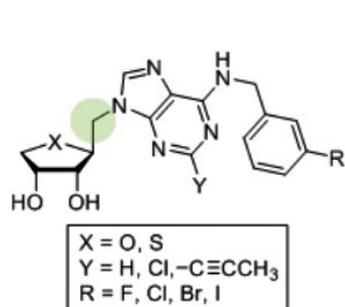
Chair: Sang Min Lim (KIST)

Synthesis and Structure-Activity Relationships of Conformationally Locked Truncated 1'-Homologated (*S*)- and (*N*)- Methanocarba Nucleosides as Dual PPAR γ / δ Modulators

Young Eum Hyun, Lak Shin Jeong*

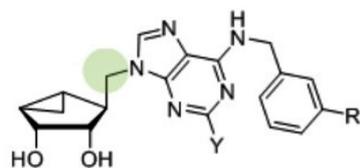
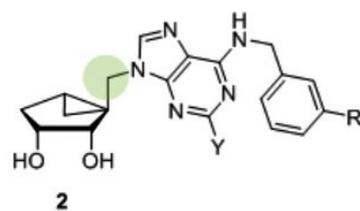
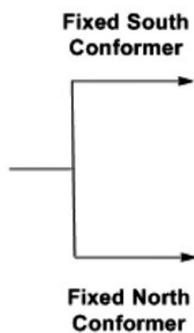
Department of Pharmacy, Seoul National University, Korea

We recently reported that novel peroxisome proliferator-activated receptor (PPAR) γ / δ dual modulators (**1**), which function as both PPAR γ partial agonists and PPAR δ antagonists, have therapeutic potential against cancer and metabolic diseases associated with hypoadiponectinemia. It is well known that the normal ribose ring of nucleosides is in a dynamic north (*N*)/south (*S*) equilibrium in the solution state. Since the energy barrier between this equilibrium is less than 6.2 Kcal/mol, it has been very difficult to confirm whether the *N* or *S* conformation is suitable for proper binding to the target enzyme or receptor for maximal biological activity. It is also widely known that bicyclo[3.1.0]hexane nucleosides locked in either north or south conformations were utilized to confirm which conformation was favorable for cellular thymidine kinase or HIV reverse transcriptase. Based on the interesting biological activity of **1** acting as PPAR γ / δ dual modulators, we wanted to identify what conformation is more favorable for binding to PPAR γ / δ . To achieve this goal, we adopted a bicyclo[3.1.0]hexane template to restrict sugar pucker. Thus, we designed and synthesized conformationally rigid southern C3'-exo conformer **2** and northern C3'-endo conformer **3**, using a bicyclo[3.1.0]hexane carbasugar. These analogs were assayed to determine their binding affinities to PPARs. Synthesis and binding affinities will be presented in detail.



1

**Pure PPAR γ / δ dual modulator
without A $_3$ AR binding affinity**



<Jeong et al., *J. Med. Chem.* 2020, 63, 16012.>



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

Oral Presentation of Young Medicinal Chemists

Room 306 (Live Streaming) THU 09:40

Chair: Sang Min Lim (KIST)

The case study on the DYRK1A inhibitor using the Topological Water Network-ligand shape similarity analysis

Hye Ree Yoon, NamSook Kang*

Graduate School of New Drug Discovery and Developm, Chungnam National University, Korea

Dual-specificity tyrosine phosphorylation-regulated kinase 1A (DYRK1A) is a protein kinase with diverse functions in cell regulation. Abnormal expression and activity of DYRK1A contribute to numerous human malignancies, Down syndrome, and Alzheimer's disease. This study describes the process of identifying DYRK1A inhibitors as a case study of our research method. Molecular dynamics (MD) simulations were performed to obtain the dynamics properties of water molecules in active site of target protein. Water molecules form water-ring networks through hydrogen bonds, which the authors have termed topological water networks (TWNs). For TWN analysis, we divided the ATP binding site into five regions (A-E) according to the binding mode of staurosporine, known as a pan kinase inhibitor. DYRK1A showed 40.5% TWN in the C region, and GSK3 β confirmed that the binding site similarity was low with DYRK1A, but the distribution of water molecules in the C region was high at 36.4%. Recently, DYRK1A was found to be associated with human pancreatic β -cell proliferation. Both DYRK1A and GSK3 β are negative regulators of the NFAT pathway, and this pathway is fundamentally important for β -cell proliferation. Shape similarity was calculated using the ultrafast shape recognition (USR) method. In the shape similarity results between the known inhibitor of GSK3 β and the TWN of DYRK1A, we found that higher TWN-ligand shape similarity values are potent as inhibitors. Based on these results, the in-house library was screened considering the TWN-ligand shape similarity and the high proportion of the C region. The seven compounds selected in the screening were tested for activity by in vitro assay. The IC₅₀ values for compounds with TWN-ligand shape similarity values of less than 25% were not determined. In TWN-ligand shape similarity, compounds with 25-40% showed IC₅₀ values of 2.9-6.8 μ M, and compounds with 40% or more showed IC₅₀ values less than 0.5 μ M. Among the selected compounds, the TWN-ligand shape similarity value was 50% or more, but the compound whose IC₅₀ value deviated from the trend confirmed that the compound size was small. Nevertheless, these compounds have inhibitory activity, making them

suitable for use as scaffolds and require optimization. We described how to identify a DYRK1A inhibitor from another known inhibitor using the TWN–ligand shape similarity method. As a computational drug discovery method, we propose the TWN–ligand shape similarity method through TWN analysis as a way to rapidly identify compounds amenable to drug repositioning.



Oral Presentation : **MED1.O-6**

Oral Presentation of Young Medicinal Chemists

Room 306 (Live Streaming) THU 09:50

Chair: Sang Min Lim (KIST)

Structural derivatives of Amyloid- β probes as new CNS penetrant histone deacetylase inhibitors

Khan Hashim Ali, Young Ho Seo^{1,*}

College of pharmacy, Keimyung University, Korea

¹*College of Pharmacy, Keimyung University, Korea*

A series of compounds with benzoheterocyclic moiety were designed, synthesized and evaluated biologically for their potential as histone deacetylase (HDAC) inhibitors that could penetrate CNS. Compound 9b, among the entire series, showed noteworthy, dose and time-dependent, potential against cellular proliferation of SH-SY5Y cells ($GI_{50} = 2.01 \mu\text{M}$) that was better than the reference drug SAHA ($GI_{50} = 2.90 \mu\text{M}$). Furthermore, 9b also enhanced the acetylation of Histone H3 and α -tubulin through HDAC1 and HDAC6 inhibitory mechanism. The in-vitro enzyme assay with compound 9b revealed IC_{50} values of 84.9 nM and 95.9 nM with HDAC1 and HDAC6 respectively. The capacity of SH-SY5Y cells to undergo colony formation was also found to be resisted in the presence of 9b, thus, indicating typical anti-carcinogenic and anti-metastatic potential of the compound. Upon comparison against SAHA for blood-brain barrier (BBB) permeation, 9b was observed to possess much stronger ability to cross BBB via theoretical prediction, in-vitro PAMPA-BBB assay and in-vivo brain pharmacokinetic experiments. The compound 9b was also docked in-silico into the substrate binding pockets of HDAC1 and HDAC6 isoforms to confirm the protein-ligand fitting. In conclusion, the synthesized compound 9b presented a novel scaffold for the development of HDAC inhibitors with ability work in the CNS.

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

Oral Presentation for Young Material Chemists

Room 405 (Live Streaming) THU 09:00

Chair: Hui-Seon Kim (Inha University)

Lattice Engineering Way to Control the Defect and Stacking Structure of Inorganic Nanosheets for Optimizing Their Electrochemical Functionalities

Tae-Ha Gu, Xiaoyan Jin¹, Seong-Ju Hwang^{1,*}

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

¹Department of Materials Science and Engineering, Yonsei University, Korea

An effective chemical way to optimize the electrochemical functionalities of layered inorganic solids is developed by controlled restacking of exfoliated 2D nanosheet (NS). The fine-control of the stacking number and oxygen defect of restacked inorganic NSs with positive layer charge can be achieved by employing diverse anions as intercalants with various ionic sizes and charge densities. The self-assembly of layered double hydroxide (LDH) NSs with low-charge-density intercalant ion like NO_3^- is quite effective in creating oxygen vacancies near redoxable metal ion and lowering stacking number. The defect-rich Co-Al-LDH- NO_3^- nanohybrid shows excellent performances as oxygen electrocatalyst and supercapacitor electrode with huge specific capacitance of $\sim 2230 \text{ F g}^{-1}$ at 1 A g^{-1} . Furthermore, the lowering of the stacking thickness caused by weakened interlayer interactions with low charge-density ions improves the charge transfer kinetics and ECSAs of the restacked LDH NSs. The present study highlights that the controlled restacking of exfoliated inorganic NSs with intercalant ions can provide an effective way to optimize its electrochemical functionalities.

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

Oral Presentation for Young Material Chemists

Room 405 (Live Streaming) THU 09:10

Chair: Hui-Seon Kim (Inha University)

Monolayered g-C₃N₄ Nanosheet as an Emerging Cationic Building Block for Strongly-Coupled 2D Superlattice Bifunctional Catalysts

Namhee Kwon, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

New class of 2D superlattice nano hybrids of interstratified graphitic-carbon nitride (g-C₃N₄)-transition metal dichalcogenide monolayers are synthesized by employing pH-controlled g-C₃N₄ nanosheet (NS) as an emerging cationic building block. The interstratification of g-C₃N₄ and MoS₂ NSs leads to the enhancement of interfacial electronic coupling between wide 2D surfaces, the creation of nitrogen vacancy, and the stabilization of 1T'-MoS₂ phase. The layer-by-layer-ordered g-C₃N₄-MoS₂ superlattice nano hybrids display remarkably improved bifunctionality as photocatalysts for visible light-induced N₂ fixation and electrocatalysts for hydrogen evolution reaction. This is attributable to the promotion of proton adsorption, the improvement of charge separation, the provision of active defect sites with enhanced N₂ molecule activation ability, and the enhancement of visible absorptivity, charge separation, and charge transfer kinetics. The present study highlights that the application of exfoliated g-C₃N₄ NS as a cationic building block provides valuable opportunity to widen the library of multifunctional NS-based superlattice nano hybrids.

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

Oral Presentation for Young Material Chemists

Room 405 (Live Streaming) THU 09:20

Chair: Hui-Seon Kim (Inha University)

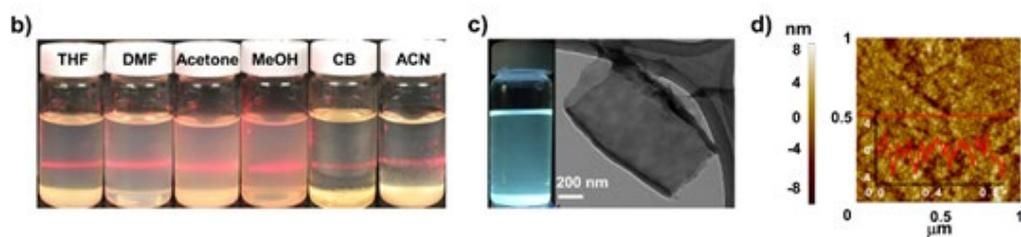
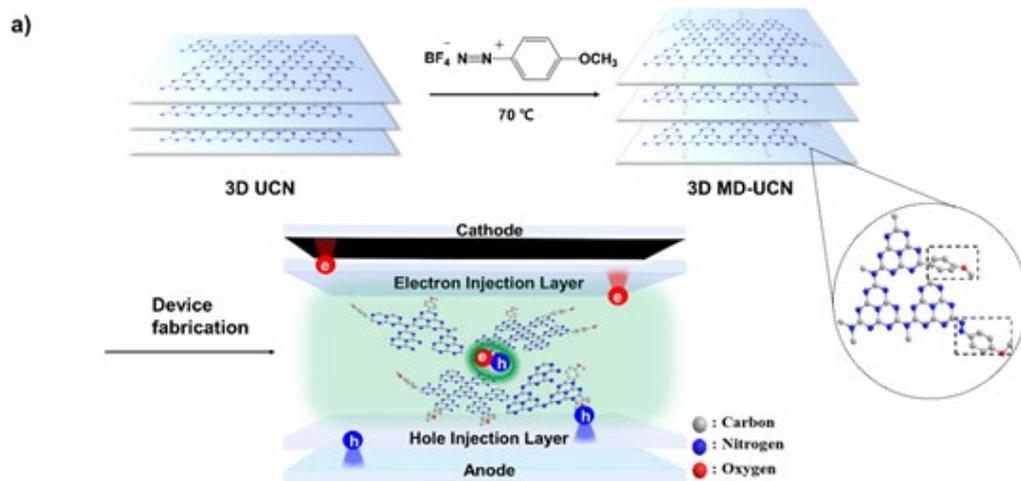
Production of Covalent Modification 2D C₃N₄ using diazonium salt and Their Electroluminescence Performance

Sunghee Park, Sungjin Park^{1,*}

Department of chemistry, Inha University, Korea

¹*Department of Chemistry, Inha University, Korea*

Carbon nitrides (C₃N₄) have a potential to optical and optoelectronic applications. However, their application to electroluminescence (EL) devices is limited by the lack of production methods of homogeneous dispersions in organic solvents owing to their rigid bulk structures, which are critically required for device fabrication. Herein we propose a strategy to generate stable dispersions of fluorescent, two-dimensional (2D) C₃N₄ materials and demonstrate light-emitting diodes (LEDs) based on them. The treatment of urea-driven C₃N₄ (UCN) with methoxy-benzene diazonium salt (MD) produces dispersions in organic solvents. Experimental and theoretical study suggests that the MD treatment passivates the surface defects of the UCN. The resulting LED devices show bright green light with promising EL performance and external quantum efficiency of 0.91%. This unprecedented result will open an era of C₃N₄ emitters as future promising light-emitters in displays and solid-state lightings.



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

Oral Presentation for Young Material Chemists

Room 405 (Live Streaming) THU 09:30

Chair: Hui-Seon Kim (Inha University)

Which is better precursor for synthesis of 3D graphene-like zeolite-templated carbon: ethylene vs propylene?

Hongjun Park, Ryong Ryoo*

Center for Nanomaterials and Chemical Reactions, Institute for Basic Science, Korea

Zeolite, a family of crystalline microporous aluminosilicate minerals, has been used for a long time as a hard template for the synthesis of three-dimensionally nanoporous carbon materials comprised of graphene-like frameworks. The zeolite-templated carbon (ZTC) materials are generally synthesized using some large-pore zeolites (e.g., FAU, EMT, and beta types) and various hydrocarbons as a carbon precursor. The ZTCs attracted great attention due to their high specific surface area, large pore volume, and electrical conductivity, which was useful for electrical energy storage applications. In this presentation, we show the results of the comparative evaluation with ethylene and propylene as the representative carbon source for the ZTC synthesis. Resultant carbon materials were characterized by X-ray powder diffraction and argon gas adsorption, to reveal the difference in carbon quality. Interestingly, there were remarkable differences between the ethylene- and propylene-derived ZTCs, depending on the zeolite framework type and the silicon-to-aluminum ratio of the template. The ZTC electrodes exhibited specific capacitances of 200-700 $F g^{-1}$ at 0.1-1 $A g^{-1}$ in an aqueous electrolyte, demonstrating a positive correlation between supercapacitance and the specific surface area.

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

Oral Presentation for Young Material Chemists

Room 405 (Live Streaming) THU 09:40

Chair: Hui-Seon Kim (Inha University)

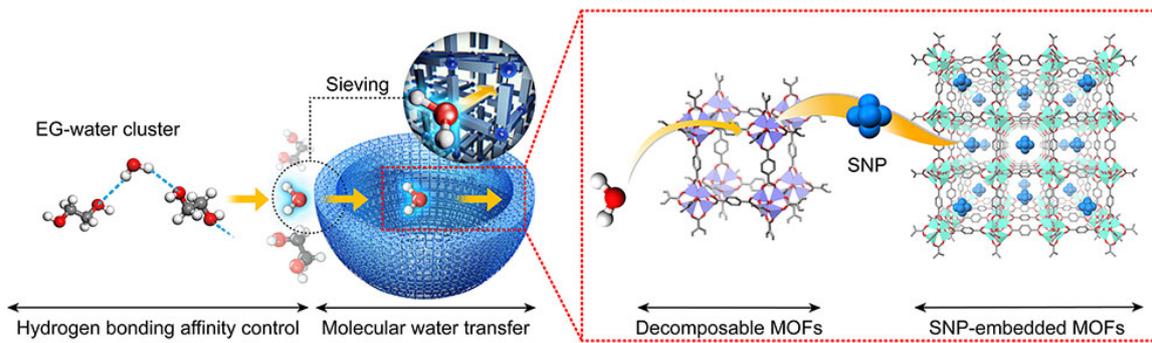
Atomic particles driven by metal organic framework with finely controlled hydrogen bonding affinity

Wonho Choi, Kyung Min Choi^{1,*}

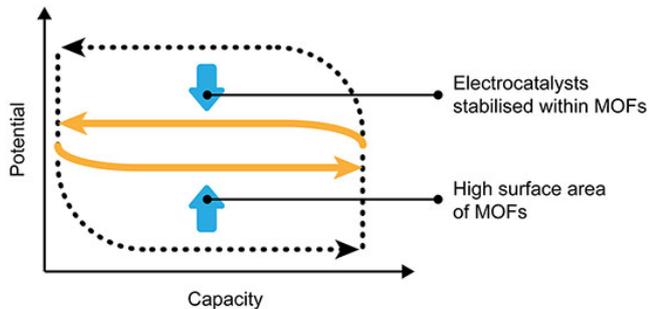
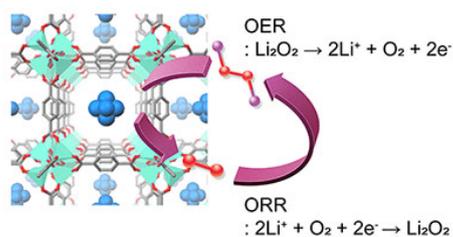
Advanced material system institute, Sookmyung Women's University, Korea

¹*Division of Chemical and Biomolecular Engineering, Sookmyung Women's University, Korea*

In principle, atomic particles can serve as enablers in full atom-to-atom reactions for many applications such as electrochemical energy conversion. However, precise control over the synthesis of atomic particles has not been successful and remains as a big challenge due to their unsaturated surface bonds typically stabilized through agglomeration. Here, we show that the generation and stabilization of atomic particles can be achieved by subjecting hydrogen bonding affinity-controlled isolated water molecules to multilayer metal-organic frameworks (MOFs). First, alternating water-decomposable and -stable MOF layers are stacked in succession to construct a multilayer MOF. Then, isolated water molecules are selectively sieved through the hydrophobic micropores of the water-stable MOF and transferred one by one to the water-decomposable MOF. This process makes it possible to transform a multilayer MOF into an atomic particles-embedded multi-shell hollow MOF. In addition, it shows that controlling the penetration of isolated water molecules is a key factor in the production of atomic particles. We chose two zeolitic imidazolate frameworks (ZIFs) as MOF structures and built multilayer MOFs up to 10 layers of water-decomposable ZIF-67 and water-stable ZIF-8 structures. By increasing the number of MOF shells, we discovered that atomic particles are highly loaded and enable remarkable performance in the cathode of a Li-O₂ battery.



• Li-O₂ battery



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

Oral Presentation for Young Material Chemists

Room 405 (Live Streaming) THU 09:50

Chair: Hui-Seon Kim (Inha University)

Monolayer graphitic carbon nitride as metal-free catalyst with enhanced performance in electro-catalysis

Huiyan Piao, Goeun Choi¹, Jin-Ho Choy^{2,*}

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¹*Department of Nanobiomedical Science, Institute of Tissue Regeneration Engineering, Dankook University, Korea*

²*Department of Pre-medical Course, Institute of Tissue Regeneration Engineering, Dankook University, Korea*

The exfoliation of bulk graphitic carbon nitride ($g\text{-C}_3\text{N}_4$) into monolayer has been intensively studied to induce maximum surface area for fundamental studies, but ended in failure to realize chemically and physically well-defined monolayer of $g\text{-C}_3\text{N}_4$ mostly due to the difficulty in reducing the layer thickness down to an atomic level. It has been, therefore, remained as a challenging issue in two-dimensional (2D) chemistry and physics communities. In this study, $g\text{-C}_3\text{N}_4$ monolayer was formed by in-situ polycondensation reaction of cyanamide precursor, which was intercalated in the interlayer space of 2D mica in prior to polymerization at 550 °C. Finally, monolayers of $g\text{-C}_3\text{N}_4$ could be separated by dissolving aluminosilicate Mica layers in an acidic solution. The atomically resolved monolayer of $g\text{-C}_3\text{N}_4$ was confirmed by spectroscopic and microscopic analyses. In addition, the experimental Cs-HRTEM image was made, for the first time, which was in excellent agreement with the theoretically simulated; the evidence of monolayer of $g\text{-C}_3\text{N}_4$ in the perfect 2D limit becomes now clear from the HRTEM image of well-known orderly hexagonal symmetry with a cavity formed by encirclement of three adjacent heptazine units. Compared to the nanolayers and the bulk, the $g\text{-C}_3\text{N}_4$ monolayer showed remarkable performances in electrocatalytic activity towards oxygen reduction reaction.

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

Oral Presentation for Young Material Chemists

Room 405 (Live Streaming) THU 10:00

Chair: Hui-Seon Kim (Inha University)

Growth Model Using Monomer Diffusion Dynamics in Colloidal InAs Nanocrystals Synthesis via continuous precursor injection.

Seongmin Park, Sohee Jeong*

Department of Energy Science, Sungkyunkwan University, Korea

Highly monodisperse colloidal InAs quantum dots (QDs) stand out for NIR/IR applications such as bio-imaging, solar cell, photodetector due to their bandgap tunability of 0.8~1.8 eV stemmed from the quantum confinement effect. To synthesize monodisperse InAs QD exhibiting the optical property in NIR region, a continuous injection has been introduced. Nevertheless, synthetic efforts to increase the particle size above 5 nm are challenging by growth suppression, accompanied by secondary nucleation or interparticle ripening during growth, leading to inhomogeneity. Here, we propose a growth model for the continuous precursor injection of colloidal InAs QDs based on monomer flux. As we expected by our model, we strictly control the diffusion dynamics of monomers by tuning reaction volume, precursor concentration, and injection rate in our experiment. As a result, we synthesize the InAs QDs with a size of about 9.0-nm (1Smax of 1600 nm) with a narrow size distribution. Our control of monomer flux synthesis can effectively overcome the previous size limit of InAs nanocrystal growth.

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

Oral Presentation for Young Material Chemists

Room 405 (Live Streaming) THU 10:10

Chair: Hui-Seon Kim (Inha University)

Bioinspired Functional Coating and Adhesive

Kyueui Lee

Department of Chemistry, Kyungpook National University, Korea

Polyphenols play numerous biological roles in nature, which often gives lots of insights on developing functional materials. For example, marine mussel secretes 'sticky' polyphenols that allow to fasten the entire body of mussel to the neighboring substrate to prevent sweeping away from harsh waves. Polydopamine is a representative polymeric material that mimics the polyphenol chemistry of marine mussel (Messersmith et al., Science, 2007, 318, 426). Polydopamine shows strong adhesion toward neighboring substrates like polyphenol in mussels; thus, it can be easily deposited on virtually any kind of surface. Moreover, since polydopamine shows multifunctionality due to the unique catechol functionality, it has been adopted in various applications as an attractive surface engineering tool. However, its practical usage has been severely limited due to its inherently weak mechanical resistance. To overcome this problem, we recently developed a method where polydopamine can be partially graphitized through light-material interaction. Since graphitic material is a well-known material showing strong mechanical properties, the resultant material showed significant mechanical improvements, while its inherent functionality was still preserved. In the second part of the talk, I would like to introduce another adhesive polymer inspired by polyphenol chemistry found in marine mussels. Due to the sticky nature of polyphenols, as developed material showed strong adhesion properties. Furthermore, the adhesion between the adhesive and substrates was successfully functioning in the underwater condition, which is highly desired in the adhesive market.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 406 (Live Streaming) THU 09:35

Chair: Hye Ryung Byon (KAIST)

Scanning Electrochemical Microscopy for Better Electroanalysis

Je Hyun Bae, Michael. V Mirkin^{1,*}

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

¹Department of Chemistry and Biochemistry, Queens College, United States

Electroanalytical methods are a class of analytical methods which study analytes by measuring the electrical properties in an electrochemical cell containing analytes. These methods have been widely used because of relatively simple and inexpensive techniques, low limit of detection, and measurement of electrically original signals. With the development of nanotechnology, electroanalysis has been advancing and offers new opportunities in analysis. In this talk, I will introduce Scanning Electrochemical Microscopy (SECM) as a nanoelectroanalytical tool used in our research. SECM is a scanning probe microscopy to measure the local electrochemical behavior of interfaces. Our efforts for electroanalysis at the nanoscale with SECM will be presented.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 406 (Live Streaming) THU 10:00

Chair: Hye Ryung Byon (KAIST)

Unraveling thermoelectric properties by electrochemical impedance spectroscopy

Chung-Yul Yoo

Department of Chemistry, Mokpo National University, Korea

Impedance spectroscopy has been widely used in the field of energy storage materials since the analysis of the impedance spectrum enables the investigation of elementary electrochemical reaction of electrode, electrolyte, electrode/electrolyte interfaces to understand and develop battery, fuel cell, and supercapacitor materials. Recently, the electrochemical impedance spectroscopy measurements enable the determination of three key parameters-the Seebeck coefficient, thermal conductivity, and electrical conductivity-by employing a one-dimensional heat equation [1-3]. This presentation focuses on the theory, data validation, and applications of electrochemical impedance spectroscopy in order to interpret the thermoelectric devices. The effects of operating condition of devices on the impedance spectroscopy data discussed in detail. [1] Yoo et al., Applied Energy, 251, 113341 (2019).[2] Yoo et al., Journal of Electronic Materials, 48, 1833 (2019).[3] Yoo et al., Energy, 152, 834 (2018).

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

Oral Presentation of Young Scholars in Electrochemistry

Room 406 (Live Streaming) THU 10:25

Chair: Hye Ryung Byon (KAIST)

A Study of Electrochemical Olefin Epoxidation

Kyoungsuk Jin

Chemistry Department, Korea University, Korea

Over several decades, electrochemistry has played an imperative role in synthetic chemistry. Although electrochemical organic synthesis can be driven with environmentally-friendly sources of electricity, only a small number of commodity chemicals have been produced via electrochemical reactions; namely, anthraquinone, some perfluorinated hydrocarbons, and adiponitrile, a key intermediate for the polymer Nylon 6,6. Most research into these synthetic approaches is just at the laboratory scale. The fact that such minimal attention has been paid to the commercialization of these methods has been attributed to high energy costs due to the required large overpotential values and poor selectivity toward desired products. In this regard, we need to focus on addressing challenging electro-organic synthesis problems through engineering efficient catalysts and gaining a deeper understanding of reaction mechanisms on those catalysts. In this talk, I will present our recent studies about electrochemical olefin epoxidation by using manganese oxide nanocatalysts. Epoxides are useful intermediates for the manufacture of a diverse set of chemical products. Current routes of olefin epoxidation either involve hazardous reagents or generate stoichiometric side products, leading to challenges in separation and significant waste streams. Recently we demonstrated a sustainable and safe route to epoxidize olefin substrates using water as the oxygen atom source at room temperature and ambient pressure. Electrokinetic studies provided insights into the mechanism of olefin epoxidation, including an approximate first-order dependence on the substrate and water and a rate-determining step that involves the first electron transfer.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 406 (Live Streaming) THU 11:00

Chair: Hye Ryung Byon (KAIST)

Self-standing Electrodes for High-temperature PEMFCs fabricated by Electrospinning

Sung Yul Lim, Santiago Martin¹, Shao Jing^{2,*}, Wenjing Zhang^{3,*}

Department of Chemistry, Kyung Hee University, Korea

¹*National University of Distance Education, Department of Mathematical and Fluid Physics, Spain*

²*College of Chemistry and Environmental Engineering, Shenzhen University, China*

³*Department of Environmental Engineering, Technical University of Denmark, Denmark*

In PEM fuel cells (PEMFCs), structuring catalysts in membrane-electrode assemblies (MEAs) is imperative for the highly efficient electrochemical conversion of O₂ gas into H₂O with less Pt-group metal loading. In addition, the generated H₂O at the active sites should be effectively removed for the large influx of O₂. The nanofibrous catalysts with continuous network of submicron 1D structure is beneficial for satisfying these conditions, which leading to the high performance. In this regard, electrospinning is one of the most promising technique to fabricate the nanofibrous catalysts for PEMFCs with scalability. Not only for structuring the catalysts in submicron dimensions, but also multi-scale design tunability is bestowed by employing the nanomaterials as the constituents of electrospun fibers. Herein, nanofibrous catalyst film prepared by electrospinning for high-temperature PEMFCs (HT-PEMFCs) will be presented. The catalyst based on interconnected fibers is flexible, consisting of Pt-Co active sites which derived from hollow zeolitic imidazolate framework. Owing to the flexibility, the catalyst layer is directly transferred to form MEA without any spray-based coating or hot-press procedures which can cause severe damage or loss of the catalysts. Our self-standing electrodes exhibit good stability in an HT-PEMFC single cell measurements, that is exceptional phenomena for other Pt-transition metal alloy catalysts at 160 °C of HT-PEMFC operation condition.

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

Oral Presentation of Young Scholars in Electrochemistry

Room 406 (Live Streaming) THU 11:25

Chair: Hye Ryung Byon (KAIST)

Electrochemistry: When small is big

Dong Young Chung

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

One of the characteristics of electrochemistry can be defined as ‘When small is big’. During an electrochemical reaction, there is an opportunity for trace level of impurities to arise from the materials to the experimental setup. Not surprisingly, this type of impurity problem has been commonly observed in various electrochemical reactions including oxygen reduction/evolution reaction, hydrogen oxidation/evolution reactions. While these studies have helped to develop a conceptual understanding of the role of impurities, many key questions are still difficult to grasp, especially when the trace level of impurities are present in electrochemical interface. In this talk, I will discuss how a small amount of an impurity can change all trends of activity and stability in the water electrolysis-oxygen evolution reaction (OER). Based on the fact that a small amount of Fe in the electrolyte can completely change the reaction kinetics of OER activity as well as OER stability, the importance of dynamic electrochemical interface and its design will be discussed.

Award Lecture in Division : **ENVR.O-5**

General Session (inc. Award lecture)

Room 302 (Live Streaming) THU 10:00

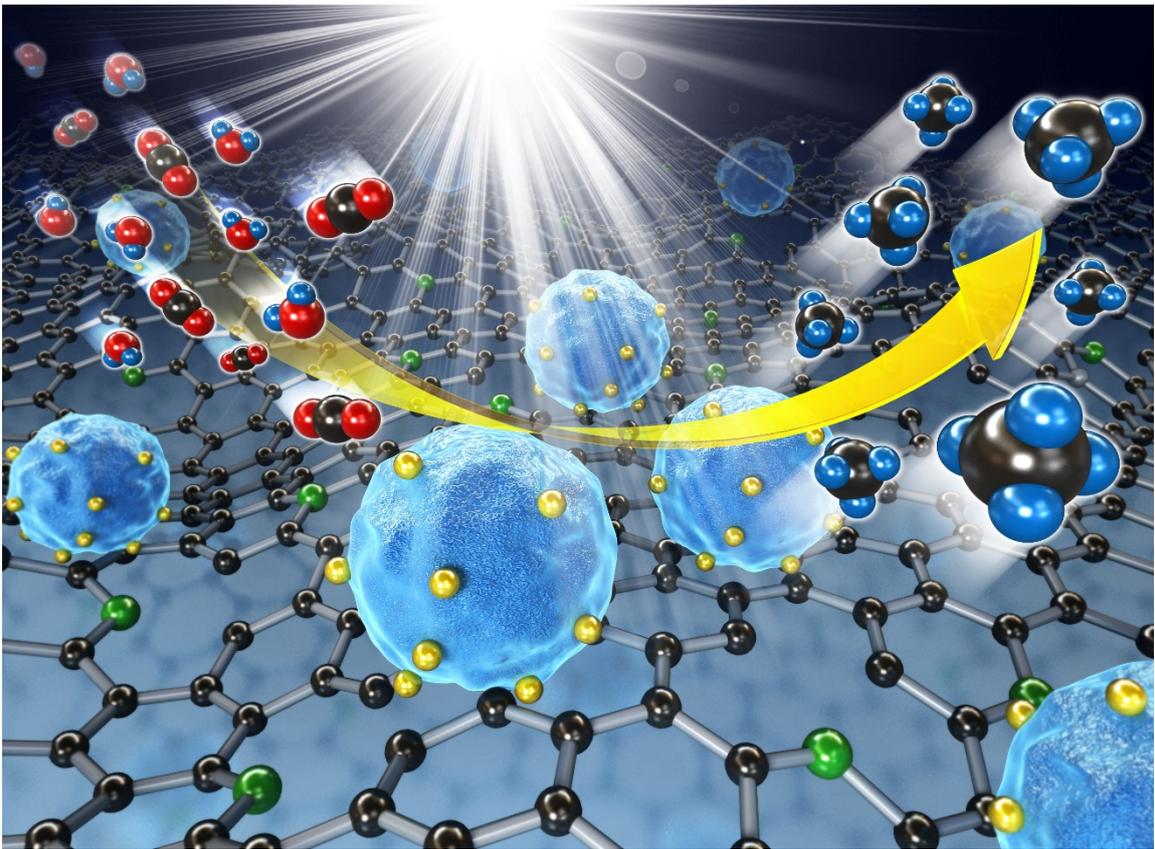
Chair: Kiyoung Lee (Kyungpook National University)

Solar Powered Chemistry: Research and Development Strategy to Accelerate Photocatalytic CO₂ Reduction

Su il In

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

A desire for renewable alternatives to fossil fuels can be achieved by utilizing CO₂, H₂O, and solar energy to generate solar fuels. A novel N-doped graphene oxide enfolded reduced titania (NGO-RT) composite was demonstrated for photocatalytic CO₂ reduction into CH₄. Later, a small amount of Pt NPs was deposited on NGO-RT that increases the catalytic performance towards CH₄ formation. The optimized Pt1.0%-NGO-RT catalyst displayed a selective visible-light CO₂ reduction into CH₄ using a flow reactor system with ≈ 12 and ≈ 2 times higher activity than pristine RT and NGO-RT, respectively. The catalyst demonstrated long-term stability over 35 h. The photo-induced CO₂ reduction mechanism was first validated through the electron transfer process, where charge trapping by Ti³⁺ states near the conduction band of RT plays a vital role in the selective CH₄ evolution. These trapped electrons transfer from RT to the closely connected interface of N-doped graphene oxide and Pt NPs to restrict the recombination of electron/hole pair. The improved catalytic performance can be attributed to RT's downward band bending at the NGO-RT interface, where electron transfer from RT to NGO decreases the charge recombination.



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

General Session (inc. Award lecture)

Room 302 (Live Streaming) THU 09:00

Chair: Kiyoung Lee (Kyungpook National University)

Application of novel Pd-In bimetallic catalyst supported by kaolin-derived zeolite for nitrate removal in real groundwater

Minhee Choi, Sunho Yoon, Sungjun Bae^{1,*}

Environmental engineering, Konkuk University, Korea

¹*Department of Environmental Engineering, Konkuk University, Korea*

In this study, we developed a novel Pd-In bimetallic catalyst supported by kaolinite induced zeolite (ZK) for efficient nitrate (NO_3^-) reduction in groundwater system. ZK was synthesized at different crystallization temperature. Among the temperature examined in this study, ZK was completely synthesized as Na-Y zeolite at 70°C (ZK70). Pd-In bimetallic catalyst supported by ZK70 showed higher NO_3^- removal and N_2 selectivity than that of other Pd-In bimetallic catalysts supported on commercial materials such as raw kaolin, silica, alumina and C-4A zeolite. From diverse surface analysis, we confirmed that the rejuvenation of In by active H species on Pd surface is the key factor that controls the enhanced NO_3^- reduction and high N_2 selectivity. Applying the optimized Pd-In/ZK70 catalyst to NO_3^- contaminated groundwater and control experiments using deionize water revealed that the catalytic activity was significantly affected by various constituents in groundwater. Especially, the results from fluorescence excitation emission matrix spectroscopy (FEEM) showed that humic-like and fulvic-like organic substances potentially inhibited the catalytic NO_3^- reduction. As well as, some dissolved inorganic ions (i.e., Cl^- , SO_4^{2-} , and Ca^{2+}) inhibited the catalytic NO_3^- reduction through different inhibitory mechanisms. The results from this study demonstrate the potential applicability of kaolinite induced zeolite (ZK) as a support of bimetallic catalyst for effective catalytic denitrification, highlighting the influence of organic and inorganic substances present in groundwater on the catalytic activity of bimetallic catalyst. Acknowledgments This research was supported by the Korea Environment Industry & Technology Institute (KEITI) through “Subsurface Environmental Management (SEM) Project”, funded by Korea Ministry of Environment (MOE) (2020002480006)

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

General Session (inc. Award lecture)

Room 302 (Live Streaming) THU 09:15

Chair: Kiyoung Lee (Kyungpook National University)

Cellulose nanocrystals coated with a tannic acid-Fe³⁺ complex as a significant medium for efficient CH₄ microbial biotransformation

Hwa Heon Je, Dong Soo Hwang*

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

Microbial biotransformation of CH₄ gas has been attractive as a sustainable and clean process for the production of energy and high-value chemicals. However, insufficient supply of CH₄ in a microbial medium due to mass-transfer limitations and the low solubility needs to be overcome for the efficient utilization of CH₄ biotransformation processes. Here, we utilized cellulose nanocrystals coated with a tannic acid-Fe³⁺ complex (TA-Fe³⁺+CNCs) as a component of a microbial medium to prepare a biocompatible nanofluid for enhancing gas-liquid mass-transfer performance. TA-Fe³⁺+CNCs were well suspended as an appropriate nanofluid component in water without any agglomeration, and an increased concentration of TA-Fe³⁺+CNCs increased the CH₄ solubility by 20% and the k_{La} value at a rapid inlet gas flow rate. Moreover, the cell growth rate of *Methylomonas* sp. DH-1 as model CH₄-utilizing bacteria improved with TA-Fe³⁺+CNC concentration without any cytotoxic or antibacterial properties. These results showed that TA-Fe³⁺+CNCs could be utilized as a significant component in the culture medium and that the TA-Fe³⁺+CNC nanofluid could be applicable as a promising medium for efficient CH₄ microbial biotransformation.

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

General Session (inc. Award lecture)

Room 302 (Live Streaming) THU 09:45

Chair: Kiyoung Lee (Kyungpook National University)

Solar photocatalytic reduction of CO₂ to hydrocarbon utilizing TiO₂ NT arrays decorated with GQDs

Dongyun Kim, Su Il In*

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

TiO₂ nanotube arrays (TNT) offer an exciting prospect as a photocatalytic material architecture due to the combined properties of high surface area, 1-D vectorial charge transfer, and reduced charge recombination. However, the large bandgap of TiO₂ (≈ 3.2 eV) limits light absorption to the UV region, which comprises but a small fraction of the solar spectrum energy. Graphene is known to effectively absorb visible light, and its high conductivity promotes efficient charge transfer. Herein, we present a novel photocatalyst composed of TNTs sensitized with electrodeposited graphene quantum dots (GQDs). GQDs electrodeposition-duration is varied to optimize photocatalytic the performance of the resulting nanostructured graphene-TNT (G-TNT) films. Under solar spectrum illumination, we find optimal G-TNT samples promote a CO₂ to CH₄ photocatalytic conversion rate of 1.98 ppm cm⁻² h⁻¹.

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

General Session (inc. Award lecture)

Room 302 (Live Streaming) THU 09:93

Chair: Kiyoung Lee (Kyungpook National University)

Formation of Durable Triple Phase Boundary in Porous Catalyst Layers for Hydrogen Evolution

Jong-Hyeok Park, Jin-Soo Park^{1,*}

Department of Civil, Environmental, Korea

¹*Department of Green Chemical Engineering, Sangmyung University, Korea*

Water electrolyzers require the movement of ions generated and consumed at two electrodes, i.e., anode and cathode. Ions should be transported inside electrodes to participate in anodic and cathodic reactions. Much efforts have been devoted to develop quasi-solid electrolytes such as gel polymer, ion exchangeable polymers, impregnation of ions in porous matrix and so on. Among the candidates, ion exchangeable polymers are quite often chosen as ion conducting media for energy conversion devices. The technique to introduce ion exchangeable polymers within electrodes for oxidation and reduction reactions is to solidify catalyst inks consisting of electrocatalyst, dispersion of ion exchangeable polymers, controlling solvents and additives by evaporation of all solvents in catalyst inks. Ion exchangeable polymers could be dispersed in various solvents. It causes different shapes of ion exchangeable polymers in solvents, for instance, cylindrical rods, a less-defined large particles, coils and so on. Such different types of ion exchangeable polymers form distinguished structure catalyst layers. In this study, the effect of solvents dispersing ion exchangeable polymers 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. Acknowledgment This research was supported 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).

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

New Trends in Chemistry Education

Room 302 (Live Streaming) THU 13:00

Chair: Seoung-Hey Paik (Korea National University of Education)

Analysis of Science Teachers' Student Assessment Status According to Online Classes

Sungki Kim

Korea Institute for Curriculum and Evaluation, Korea

The school scene in 2020 has undergone many changes due to Corona 19, which hit the world. Many scholars predict that even if Corona 19 ends, the parallel online and offline will continue in the future. In this situation, as online classes were held in 2020, the status of student assessments by science teachers was investigated. As a result of the survey, many science teachers had difficulty in conducting assessment in a online learning environment due to the reliability and fairness of the assessment. They also talked about the lack of ability to design student assessments in an online environment. Integrating this, I would like to suggest a plan to further promote online student evaluation in a blended educational environment.

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

New Trends in Chemistry Education

Room 302 (Live Streaming) THU 13:15

Chair: Seoung-Hey Paik (Korea National University of Education)

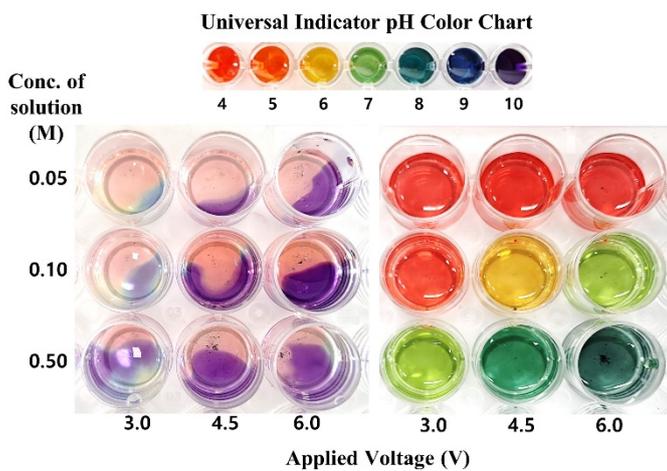
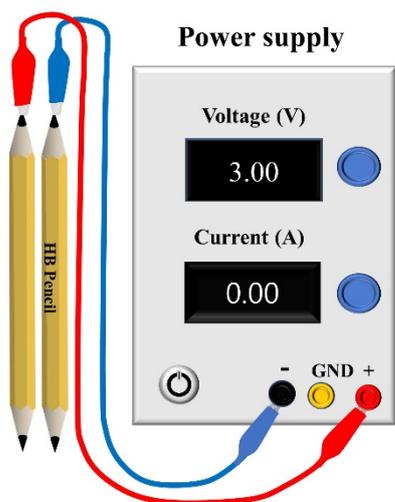
Utilizing unexpected results in water electrolysis to engage students in scientific inquiry

Kihyang Kim, Seounghey Paik^{1,*}

Chemistry, Sejong Academy of Science and Arts, Korea

¹*Department of Chemical Education, Korea National University of Education, Korea*

Water electrolysis, a well-known and simple experiment, confirms that a water molecule comprises hydrogen and oxygen atoms. In this experiment, hydroxide or hydrogen ions generated from each electrode were identified using an indicator based on the assumption that electrodes, electrolytes, and indicators do not participate in the water electrolysis reaction. However, KNO_3 , which is considered as an electrolyte that is non-reactive during water electrolysis when considering the standard reduction potential, can affect electrolysis. Pencil graphite electrodes, which are commonly used in student experiments because of their low cost and easy availability, and indicators used to identify the products of water electrolysis can also influence this reaction. Therefore, students can observe various anomalies during the water electrolysis experiments. We have developed an experimental activity that allows students to observe anomalous phenomena in water electrolysis experiments. By performing this water electrolysis activity, students can participate in the process of scientific inquiry, create models, design their own research processes, conduct experiments, analyze and interpret data, and formulate evidence-based arguments based on the results of the proposed activity. By engaging in this activity, students can realize that water electrolysis is a complex process and is affected by a range of conditions.



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

New Trends in Chemistry Education

Room 302 (Live Streaming) THU 13:15

Chair: Seoung-Hey Paik (Korea National University of Education)

An Analysis for Gender-Role Stereotype of Illustrations in Middle School Science Paper Textbooks and Digital Textbooks Developed under the 2015 Revised National Curriculum

Nayoon Song, Taehee Noh*

Department of Chemistry Education, Seoul National University, Korea

This study analyzed illustrations of middle school science paper textbooks and digital textbooks under the 2015 revised national curriculum in the aspect of gender-role stereotype. Both paper and digital textbooks showed the highest frequency of multiple pupils. For pupils, both paper and digital textbooks showed similar gender rates regardless of grade. In both paper and digital textbooks, learning activities presented girls more frequently, the opposite tendency presented in non-learning activities. Both paper and digital textbooks were portrayed positively regardless of gender, and the gender rates were similar. For adults, both paper and digital textbooks showed higher frequency of men regardless of grade. In both paper and digital textbooks, housework activities were balanced by gender, but outdoor activities presented men more frequently. In both paper and digital textbooks, men appeared in a broader range of occupations than women. Paper textbooks showed a higher frequency of men, however opposite tendency showed in digital textbooks. Both well-known scientist and anonymous scientist had a higher proportion of men. In particular, digital textbooks showed a large gender imbalance in the field of education. The proportion of men was higher in all behavioral characteristics in both paper and digital textbooks.

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

New Trends in Chemistry Education

Room 302 (Live Streaming) THU 13:30

Chair: Seoung-Hey Paik (Korea National University of Education)

Comparison on Factor for Improving Positive Experiences about Science Between General Elementary School Students and Scientifically-Gifted Elementary School Students

Hunsik Kang

Elementary Gifted Education, Seoul National University of Education, Korea

The purpose of this study is to compare the factors for improving positive experiences about science (PES) between general elementary school students and scientifically-gifted elementary school students. For this study, 16 students in grades 5~6 from 4 elementary Science Core schools and 36 students in grades 5~6 at a gifted science education institutes in Seoul were selected. After weekly Saturday classes and all curriculum of the institutions were over, in-depth interviews were also conducted with the students to explore the factors for improving their PES. The analysis of the results reveal that the factors for improving PES of general and scientifically-gifted elementary school students were ‘practice-centered exploratory activities’, ‘student-led class’, ‘positive and professional feedback’, ‘construction of knowledge through exploration’, ‘class considering student’s interest and aptitude’, ‘use of materials related to real life’, ‘smooth communication and collaboration in group activities’, and ‘appropriate difficulty in learning content’. There were also six factors that only emerged from science-gifted students: ‘Learning experience through scientific creativity strategies’, ‘inquiry experience as a little scientist’, ‘advanced or accelerated learning experience’, ‘learning experience with students with similar level’, ‘experience helping other students’, and ‘experience with high or low achievement’. Based on these results, the practical implications for improving the student’s PES are suggested.

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

New Trends in Chemistry Education

Room 302 (Live Streaming) THU 14:00

Chair: Seoung-Hey Paik (Korea National University of Education)

Research ethics education through knowledge of how to write lab notes for high school students

Eun-Young Choi

Chemistry & Biology, Korea Science Academy of KAIST, Korea

We are currently witnessing a large need for education regarding research ethics, especially for Science High School conducting research. Recent events have put a spotlight on faulty research achievements of youth, and this has caused our high school's research projects to be subjected to intense scrutiny. When the honesty of a high school student project is inspected, evidence is needed that the research is actually the work of high school students. This evidence can most easily be provided through lab notes. Teachers in charge of research and high school students conducting research need to be aware of research ethics, and they should be aware of the need to write lab notes. Therefore, it is necessary to investigate the current perceptions of high school teachers and students conducting research and to make them aware of the need for research ethics. The way to adhere well to research ethics at the high school level is to understand the function of lab notebooks and write them well. Therefore, I would like to report on the details of basic research ethics that high school students need to know and how to write research notes. For Korea Science Academy of KAIST, the guidelines for writing a lab notebook were most recently finalized on September of 2020 and began to proceed our own education of research ethics and lab notes in earnest. Therefore, I would like to report KSA's lab notes education and management.

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

New Trends in Chemistry Education

Room 302 (Live Streaming) THU 14:15

Chair: Seoung-Hey Paik (Korea National University of Education)

**Analysis of Ignorance of models related to oxidation and reduction
phenomena presented in the 2009 • 2015 revised curriculum chemistry
I and chemistry II textbooks**

Eunju Ryu, Eunsun Jeon, Seounghey Paik^{1,*}

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

¹*Department of Chemical Education, Korea National University of Education, Korea*

In this study, we analyzed whether the textbook reveals the Ignorance of the electron transfer model and the oxidation state model that explain the oxidation-reduction phenomena, which are important topics in chemistry curriculum. The Ignorance of the model is the nature of the model that must be perceived for the development and use of the model among the 'practices' emphasized in the 2015 revised curriculum. It is also important in modeling. To this end, based on previous studies dealing with the Ignorance of the acid-base model, related prior studies and four general university chemistry textbooks were analyzed to extract the analysis criteria for the study. Based on this, 9 chemistry I textbooks and 6 chemistry II textbooks in the 2015 revised curriculum were analyzed. In addition, 4 types of chemistry I textbooks and 4 types of chemistry II textbooks in the 2009 revised curriculum were analyzed to compare the differences in content according to the revised curriculum. Based on the results of the analysis, a method for improving the contents of textbooks was proposed to allow students and chemistry teachers to perceived the value of Ignorance in modeling education.

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

New Trends in Chemistry Education

Room 302 (Live Streaming) THU 14:30

Chair: Seoung-Hey Paik (Korea National University of Education)

A Study on the Development and Application of Responsive Teaching Teacher Education Program for Chemistry Teachers

Jeong Soo Kim, Seounghey Paik^{1,*}

Bupyeong Girls' High School, Korea

¹*Department of Chemical Education, Korea National University of Education, Korea*

This study was conducted to enhance the teaching capacity of responsive teaching for chemistry teachers participating in programs held in the Graduate School of Education. In the study, 14 chemistry teachers participated in a 'practice-focused' responsive teaching teacher education program over a three-week period. The program was conducted in four stages. (1) Step [I]-Introduction-is a step of understanding responsive teaching and introducing examples of it, in which the teachers approach actual class cases in which responsive teaching is applied in a macroscopic way(6 hours). (2) Step [C]-Case Study-is a step of analyzing cases of responsive teaching, and learning how to analyze the application of responsive teaching from student responses(8 hours). (3) Step [D]-Discussion-is a step of deepening the understanding by discussing the cases of responsive teaching, in which teachers explore various ways of promoting students' responses through students' group assignment performance and in-depth group discussions in a given class scene(10 hours). (4) Step [A]-Application- is a step in which a responsive teaching method is applied, and by presenting a lesson scene that cause cognitive conflict, teachers establish a teaching strategy to promote student responses through group assignments(26 hours). The fundamental goal of teacher education is to provide better support for teachers to learn to use knowledge in practice. Student-centered classes can be created by the environments where students can reorganize their concepts and expand their thinking. To create the classroom teaching paradigm in which students-led thinking is expanded, the development and implementation of teacher education programs to reinforce the responsive teaching capacity of teachers are required.

Poster Presentation : **POLY.P-1**

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

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

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

Department of Chemistry, Chungnam National University, Korea

Oxygen (O₂)-mediated controlled radical polymerization was performed on surfaces under ambient conditions, enabling on-surface polymer brush growth under open-to-air conditions at room temperature in the absence of metal components. Polymerization of zwitterionic monomers (MPDSA_H) using this O₂-mediated surface-initiated reversible addition fragmentation chain-transfer (O₂-SI-RAFT) method yielded hydrophilic surfaces that exhibited anti-biofouling effects. O₂-SI-RAFT polymerization can be performed on large surfaces under open-to-air conditions. Various monomers including (meth)acrylates and acrylamides were employed for O₂-SI-RAFT polymerization; the method is thus versatile in terms of the polymers used for coating and functionalization. A wide range of hydrophilic and hydrophobic monomers can be employed. In addition, the end-group functionality of the polymer grown by O₂-SI-RAFT polymerization allowed chain extension to form block copolymer brushes on a surface.

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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

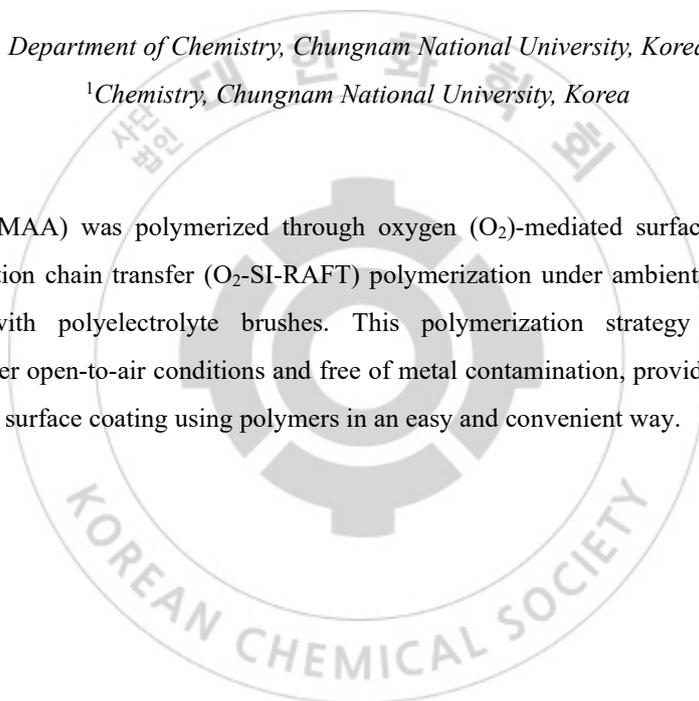
Surface-initiated RAFT polymerization of methacrylic acid under ambient conditions

Ji Hoon Lee, Seung-yeon Lee¹, Woo Kyung Cho, Kyung-sun Son*

Department of Chemistry, Chungnam National University, Korea

¹Chemistry, Chungnam National University, Korea

Methacrylic acid (MAA) was polymerized through oxygen (O₂)-mediated surface-initiated reversible addition-fragmentation chain transfer (O₂-SI-RAFT) polymerization under ambient conditions, enabling surface coating with polyelectrolyte brushes. This polymerization strategy enables on-surface polymerization under open-to-air conditions and free of metal contamination, providing an experimenter-friendly method for surface coating using polymers in an easy and convenient way.



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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Ring-opening copolymerization of cyclic epoxide and anhydride using a five-coordinate chromium complex with a sterically demanding amino triphenolate ligand

Minki Cho, Eunsung Lee^{1,*}, Kyung-sun Son^{*}

Department of Chemistry, Chungnam National University, Korea

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

An alternating ring-opening copolymerization (ROCOP) of epoxides (cyclohexene oxide, limonene oxide) and anhydrides (phthalic anhydride, naphthalic anhydride and maleic anhydride) was performed using a chromium complex containing a sterically demanding amino triphenolate ligand in the presence of a cocatalyst (bis(triphenylphosphine)iminium chloride (PPNCl) or 4-dimethyl aminopyridine (DMAP)). The polymerization reaction was strongly affected by the types and feed ratio of monomers and cocatalysts. After optimizing the reaction conditions, the chromium complex successfully produced perfectly alternating polyesters in high selectivity (> 99% ester linkages), with high molecular weights (up to 43.8 kDa), high glass transition temperatures (T_g up to 159 °C), and low dispersities. In addition, a small amount of catalyst yielded a turnover frequency (TOF) as high as 380 h⁻¹.

Poster Presentation : POLY.P-4

Polymer Chemistry

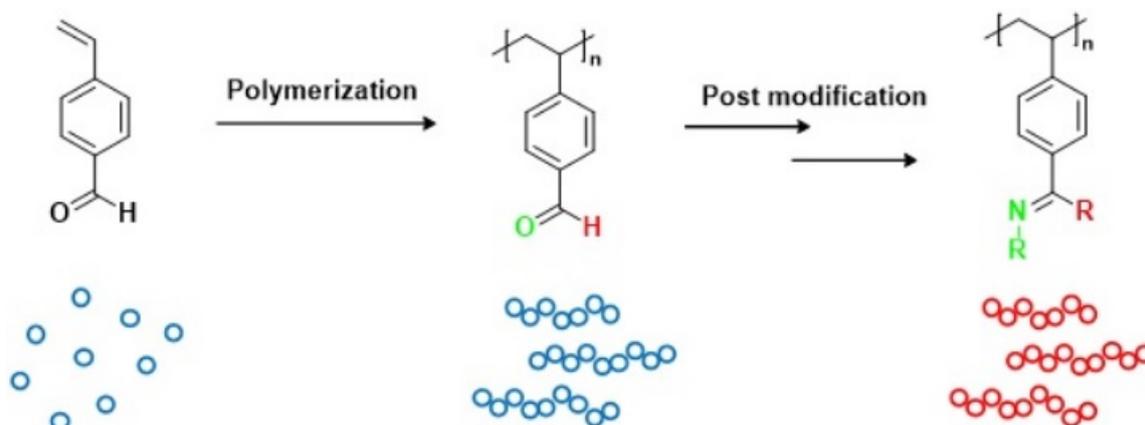
Zoom 1 FRI 15:00~16:00

Multifunctional Polymer Synthesis: Sequential Postpolymerization Modification of Aldehyde Polymers

HyoWon Lee, Jeung Gon Kim*

Department of Chemistry, Jeonbuk National University, Korea

PostPolymerization Modification(PPM) is important way to elaborating polymer performance, and PPM of polymer is one of the options for diversifying functional groups. However, finding conditions for polymerizing two or more reactive monomers, not touching other groups, and proceeding the selective modification bring on synthetic complications. In addition, the distribution of functional groups is uneven when structurally other monomers are polymerized. Synthesis and PPM of the multifunction homopolymers have emerged th detail the precision. However, the number of functional groups available is very limited. we conducted the srudy presented here to add the aldehyde group to the list of single functional groups to accommodate multiple chemical units. aldehydes, which easy to obtain and highly reactive to converted various functional groups, play important role in synthetic chemistry. here are the two step sequential operations: 1) the Rhodium catalyzed C-H activation of the aldehyde pendent through the PPM forms ketone polymers, 2) functional group condensed between ketones and amines is synthesized and discussed as a new tool for synthetic complex polymers.



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

Polymer Chemistry

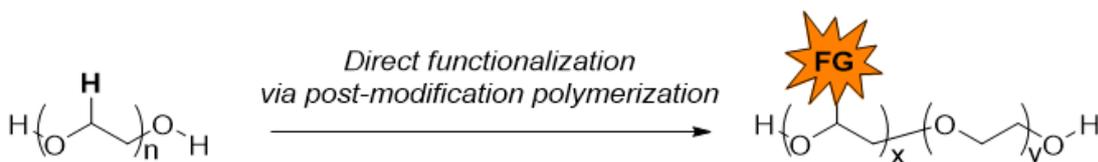
Zoom 1 FRI 15:00~16:00

Synthesis of thiolated-Poly Ethylene Glycol via Post-modification polymerization

Se Jong Kim, Jeung Gon Kim*

Department of Chemistry, Jeonbuk National University, Korea

Poly Ethylene Glycol(PEG) is hydrophilic polymer and a biocompatible polymer approve by the FDA. In addition, it is a common polymer used in battery, medicine, pharmacy and various industry. In commonly, The High-value functionalized-PEG was synthesized via pre-modification polymerization. Usually functionalized-PEG is synthesized from epoxide monomer. However, epoxide is toxic and functionalized-epoxide has limited range of monomers. as well as, it is hard to predict the reactivity of functionalized-epoxide during polymerization reaction. To overcome these limitations, the synthesis of functionalized-PEG via post-modification polymerization is preferred. In this study, Using the C-H functionalization strategy, PEG was directly functionalized using disulfide to obtain the corresponding thiolated-PEG without decreasing in the molecular weight. In conclusion, we developed an efficient post-modification polymerization methodology as a new protocol to introduce various thiolate functional groups along the polymer backbone. The detailed condition will be discussed on my presentation.



Poster Presentation : **POLY.P-6**

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Ruthenium Mediated Ring-Opening Metathesis Polymerization using Green Solvents

Eunji Hong, Jeung Gon Kim*

Department of Chemistry, Jeonbuk National University, Korea

The use of green solvents is of great interest promoting not only green metrics but also an economic benefit. While a lot of studies on the green solvent application has been conducted in most of the synthetic areas but rarely on polymerization. In this study, green solvents were evaluated for ruthenium-initiated ring-opening metathesis polymerization (Ru-ROMP) with representative monomers of norbornene, oxanorbornene and cyclooctadiene, where mostly toxic chlorinated or aromatic solvents have been used. The solvent effect was obtained by comparing the results of the reference solvent (THF, CHCl₃) and the green solvent (2-methyl tetrahydrofuran, ethyl acetate, dimethyl carbonate, and acetone). The results of all green solvents are generally promising, but chain length control was very sensitive. Among the suggested green solvents, dimethyl carbonate exhibited positive results in general.

Poster Presentation : POLY.P-7

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Co-oligomerization of 1,1-Dialkyl-3,4-diphenyl-2,5-dibromo-silole with Aromatic-diol and their Electrochemical Properties

Ji hun Lee, Young Tae Park*, Se Yeon Park¹

Department of Chemistry, Keimyung University, Korea

¹*chemistry department, Keimyung University, Korea*

Dialkyl(*iso*-propyl or *n*-hexyl)-bis(phenylethynyl)-silanes were reacted with lithium naphthalene, anhydrous ZnCl₂, and *N*-bromosuccinimide (NBS), and then the crude materials were purified to obtain 1,1-dialkyl(*iso*-propyl or *n*-hexyl)-2,5-dibromo-3,4-diphenyl-siloles, respectively. Nucleophilic substitution reactions of aromatic diols (e.g. 4,4'-biphenol or bisphenol A or 4,4'-(hexafluoroisopropylidene)diphenol) with two bromine groups of the prepared 2,5-dibromo-siloles as co-monomers in the presence of potassium carbonate under the co-solvent of *N*-methyl-2-pyrrolidinone (NMP) or *N,N*-dimethylacetamide (DMAC) and toluene with Dean-Stark trap were used to synthesize the co-oligomers containing 1,1-dialkyl(*iso*-propyl or *n*-hexyl)-3,4-diphenyl-2,5-silolene and 4,4'-biphenolene or bisphenolene A or 4,4'-(hexafluoroisopropylidene)diphenolene. The crude products are purified by decantation using deionized water. Then, it is further purified by extraction with chloroform. The product materials were characterized by not only ¹H, ¹³C, and ²⁹Si NMR but also GPC. We studied the photoelectronic properties by UV-vis absorption, excitation, and fluorescence emission spectroscopic methods, particularly, along with electrochemical properties related to lithium-ion batteries. 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-8**

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

A Study on the Manufacture and Characteristics of Porous Membrane Using Urushi Organic Gel

Jihyeon Hur, Jongok Won*

Department of Chemistry, Sejong University, Korea

The main component of natural lacquer, a catechol derivative with an alkyl chain, is polymerized into chemical bonds under the presence of Fe^{3+} ions to form urushi, while Fe^{3+} ions form an arrangement bond with the catechol group. Using this characteristic, the urushi organic gel was synthesized with a mole ratio of different concentrations of urushiol and urushiol: Fe^{3+} ions in a gamma-butyrolactone solution, and chemical bonds and distribution bonds were identified with FT-IR, respectively. From urushi organic gel, porous membrane was manufactured through freeze drying method and phase inversion method, and the correlation between porous gel and membrane porosity was studied through porous measurement and SEM. The correlation between pore structure, porosity, and mechanical strength according to the method of manufacturing pore-like membrane is considered.

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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Tough and Adhesive Milk Protein-based Hydrogel Strain Sensor for Monitoring Human-motion

Kiok Kwon^{*}, Sohyeon Heo

Korea Institute of Industrial Technology, Korea

Hydrogel is a three-dimensional polymer network structure composed of water and a polymer, and water is the major component of the hydrogel. However, high water contents of the hydrogel weaken the adhesion between hydrogel and skin, which is a bottle neck for wearable sensor application. The toughness and adhesion between hydrogel and skin is essential for body sensitive sensor application. In our research to improve the mechanical strength of hydrogel, we aim to develop a protein-based hydrogel using the milk protein sodium caseinate (SC) for high adhesion, biocompatibility, high stretchability and good toughness. In the SC-AAm hydrogel, sodium caseinate micelles and acrylamide (AAm) chains impart mechanical toughness, and hydrogen bonds enable repeated adhesion to the skin. In addition, the introduction of 2-acrylamido-2-methylpropanesulfonic acid (AMPS) imparts conductivity to the hydrogel, allowing it to act as a sensor capable of responding to various human movements such as fingers, knees, elbow bends, and deep breathing.

Poster Presentation : **POLY.P-10**

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Indacenodithienothiophene-based Conjugated Polymers for n-Channel Organic Phototransistors

Chulyeon Lee, Hwajeong Kim¹, Youngkyoo Kim^{1,*}

Department of Chemical Engineering, School of Applied Chemical Engineering, Korea

¹Department of Chemical Engineering, Kyungpook National University, Korea

Conjugated polymers have been recognized as a fascinating semiconducting material for realizing next-generation flexible and wearable devices because polymers have inherently soft and tough characteristics compared to inorganic materials. In terms of processing benefit, conjugated polymers can deliver large-area devices via solution-based roll to-roll coating on flexible plastic film substrates at low (room) temperatures. Of various organic devices, organic phototransistors (OPTRs) have attracted keen interest when it comes to their merits toward flexible detectors with active controls. Recently, a couple of conjugated polymers have been reported for the detection of both red and blue light in the geometry of OPTRs with p-channels mostly. However, both p-channel and n-channel OPTRs are necessary for advanced integrated detector systems. This presentation reports synthesis of novel n-type conjugated polymers, which are based on indacenodithienothiophene units, and their applications for n-channel OPTRs.

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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Controlling mechanical properties of liquid crystal polymer network via programmable defect arrays developed by modulation of electric field

Changjae Lee, Dong Ki Yoon^{1,*}

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

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

Mechanical properties of a polymer film required for certain application are different. In this regard, it is important to tune the properties of polymer film to have an optimized toughness or frictional force. In our work, by developing various defect arrays of mesogenic units, functional liquid crystal polymer network (LCN) film is fabricated whose tensile and frictional properties are modulated. Applying electric field with crossed electrodes generates three dimensional periodic topological defects of monomeric mixture in nematic phase. Subsequently, in-situ photo-polymerization is conducted, which results in an LCN film retaining the arrangement. Three kinds of patterns are compared in terms of mechanical properties. Increasing the number of defects in a unit area enhances toughness of the LCN film. It is the heterogeneity of elastic modulus that hinders crack propagation. Also, the film fabricated in our platform has different friction depending on the temperature. As the temperature increases, the friction coefficient of the resultant LCN film decreases, because the effective contact area is reduced due to the topographical structure change. This work suggests the strategy to increase applicability of a material for use of, for example, coating films, soft robotics, soft actuators and artificial muscles.

Poster Presentation : **POLY.P-12**

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Sequestering ATP inside Mitochondria by Nucleopeptide Assembly Induces Cancer Cell Apoptosis

Huyeon Choi, Ja-Hyoung Ryu^{1,*}

Ulsan National Institute of Science and Technology, Korea

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

Mitochondria are essential intracellular organelles involved in many cellular processes, especially adenosine triphosphate (ATP) production. Since cancer cells require high ATP levels for proliferation, ATP elimination can be a unique target for cancer growth inhibition. We describe a newly developed mitochondria-targeting nucleopeptide (MNP) that sequesters ATP by self-assembling with ATP inside mitochondria. MNP interacts with ATP strongly through electrostatic and hydrogen bonding interactions. MNP exhibits higher binding affinity for ATP (-637.5 kJ/mol) than for adenosine diphosphate (ADP) (-578.2 kJ/mol). To improve anticancer efficacy, the small-sized MNP/ADP complex formed large assemblies with ATP inside cancer cell mitochondria. ATP sequestration and formation of large assemblies of the MNP/ADP-ATP complex inside mitochondria caused physical stress by large structures and metabolic disorders in cancer cells, leading to apoptosis. This work illustrates a facile approach to developing cancer therapeutics that relies on molecular assemblies.

Poster Presentation : POLY.P-13

Polymer Chemistry

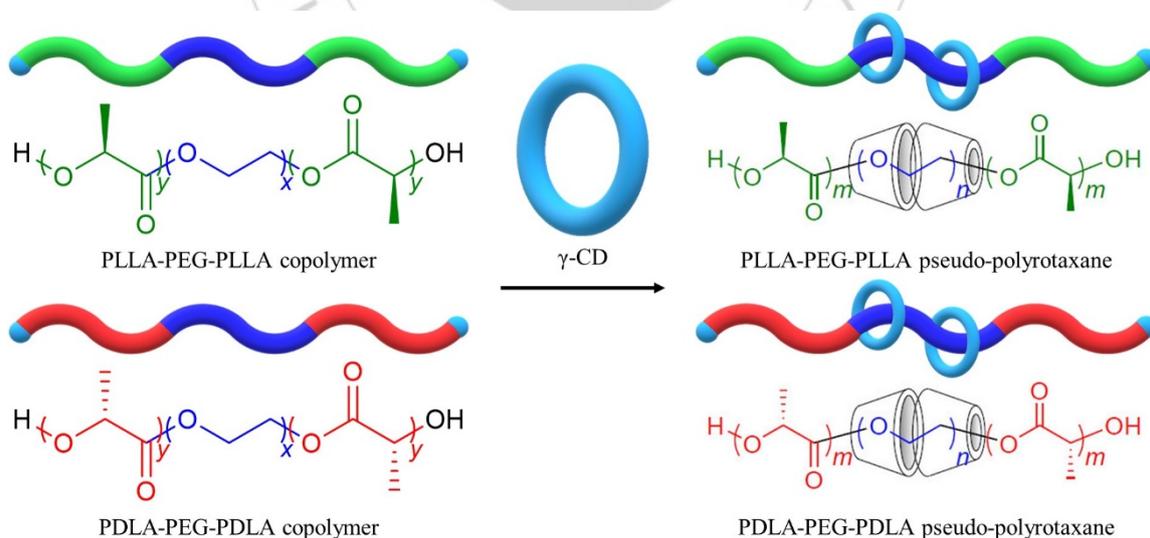
Zoom 1 FRI 15:00~16:00

Preparation of pseudo-polyrotaxane using PLA-PEG copolymer and γ -cyclodextrin and observation of its stereocomplex

Jaeyeong Choi

Division of Material Science, NAIST (Nara Institute of Science and Technology), Japan

In this study, a pseudo-polyrotaxane structure was formed by using copolymer of polylactide (PLA) and poly(ethylene glycol) (PEG) as axis components and γ -cyclodextrin (γ -CD) as wheel components. γ -CD was estimated for the inclusion of two PEG chains in one-wheel component and it was confirmed that the relationship between the obtained pseudo-polyrotaxane and γ -CD. Also, the formation of stereocomplex was confirmed by utilizing a stereoisomer of PLA which was an axis component of the obtained pseudo-polyrotaxane structure, and its characteristics were reported.



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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Colormetric strain sensor based on gold nano-particle chains embedded in thermoplastic polyurethane

Hyeon ju Ko, Seung Goo Lee*

Department of Chemistry, University of Ulsan, Korea

A battery-free colorimetric stimulus-response strain sensor is fabricated embedding linearly aggregated gold nanoparticles(i.e., gold nano-particle chain) in a thermoplastic polyurethane elastomer film. Citrate-gold nanoparticles are substituted with bis-sulfonatophenylphosphine ligand to induce linear aggregation using NaCl, and the linear length can be controlled according to the incubation time. When mechanical stress is applied to our strain sensor, a plasmonic shift is induced by the distance variation between the inter-particle of the gold nanoparticle chains, resulting in an optical response. Furthermore, by adding silica nanoparticles, moisture resistance and sensing stability are improved, also it show reversible sensing, and it is reusable by dissolving in a solvent with heat.

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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Characteristics of oxazoline based gradient and block copolymers by Langmuir-Blodgett method

Jiwon Jeong, Juraj Kronek¹, Daewon Sohn^{*}

Department of Chemistry, Hanyang University, Korea

¹Macromolecular Chemistry, Polymer Institute of the Slovak Academy of Sciences, Slovakia

Gradient and block copolymers have been synthesized by polymerization of hydrophilic 2-ethyl-2-oxazoline with hydrophobic 2-(4-octyloxyphenyl)-2-oxazoline (PEtOx-grad OctOPhOx and PEtOx-block-OctOPhOx). Poly(2-ethyl-2-oxazoline) polymers are water-soluble and biocompatible materials. Six different samples, PEtOx-grad-OctOPhOx 85/15, 62/38, 42/58, PEtOx-block-OctOPhOx 86/14, 69/31 and 55/45, have been synthesized. PEtOx-grad-OctOPhOx and PEtOx-block-OctOPhOx at the air-water interface by surface pressure (Π)-surface area (A) isotherm and Langmuir-Blodgett (LB) films of each copolymer characterized by atomic force microscope (AFM) were investigated. Surface pressure (Π)-surface area (A) isotherms show that each of copolymers has different limiting area according to the ratio between hydrophilic part and hydrophobic part. Also graphs of gradient copolymers and block copolymers show different morphologies despite similar ratios.

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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Shear-induced ordering of a lyotroped mesophase in amphiphilic random copolymer hydrogel

Minjoong Shin, Myungeun Seo^{1,*}

Chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Amphiphilic random copolymerscopolymer contains repeating hydrophilic and hydrophobic pendant groups which are randomly distributed along the polymer backbone. They Self-assemble in water ies of amphiphilic random copolymer have been studied as single chain nanoparticles (SCNP) driven by hydrophobic interaction in a diluted solution. Here, we report lyotropic behavior of their aqueous solutions in concentrated regimes. A phase window forming a physical gel is identified, where structural hierarchy across the recent progress in investigating hierarchically ordered mesophases of the amphiphilic random copolymer hydrogel in an aqueous medium at higher concentration. Structural length scales from sub-20 nanometers to several angstroms arewere observed inby both small and wide angle x-ray scattering studies(SAXS and WAXS). The mesophase can be readily aligned under shear to show anisotropy allowing us to aDynamical oscillatory shear applied in situ during the SAXS measurement indicates the ordered structure with two related multiple length scales.

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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Fabrication of Metal-Labelled Polystyrene Particles as Internal Standard for Mass Cytometry

Daewon Sohn^{*}, Yoolee Lee

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 2-stage dispersion 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-18**

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Strain-isolated stretchable substrate by the integration of rigid and soft units using interdiffusion between heterogenous pre-polymers

Dohyun Kim, Dasol Chung¹, 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*

Soft electronics is a prominent field for various industries, such as E-skins, wearable electronics, and stretchable health care systems. For the realization of soft electronic devices, the mechanically stable stretchable substrate is crucial. A general strategy for the stretchable substrate is strain-isolation, which protects the devices from mechanical stress by dissipating the stress to stretchable units. However, conventional strain-isolation strategies have limitations in the regulation of high Young's modulus contrast, low mechanical and operational stability, and high complexity of the fabrication process. Here, we report new strain-isolated stretchable substrate based on the integration of soft and rigid units using interdiffusion between pre-polymers. The pre-polymer of rigid parts successfully forms floated droplets in the soft pre-polymer unit. As a result, we realized a new strain-isolated stretchable substrate with high Young's modulus contrast. Furthermore, the substrate safely endured at 220% of elongation, and even 10000 cycles of stretching repetition at 75% of elongation. Finally, we fabrication large area micro-heater device with a 30x30 array through the printing process, which is mechanically stable at 30% of elongation.

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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Mechanical Properties of Nylon 11/Acrylic Ionomer Blends

Yoon-Gwan Jeong, Joon-Seop Kim^{1,*}

Department of Advanced Materials Engineering, Chosun University, Korea

¹Department of Polymer Science and Engineering, Chosun University, Korea

In this study, Nylon-11 and Li + neutralized random poly (methyl methacrylate-co-acrylic acid) (PMMA) ionomer and random poly (ethyl acrylate-co-acrylic acid) (PEAA) ionomer blending machines properties were measured by using UTM. The PMMA and PEAA ionomer contents in the blends were 5, 10, 20 and 30 wt%. In the case of tensile strength, the tensile strength of pure Nylon-11 and Nylon-11 / PEAA ionomer blends was similar, but that of Nylon-11 / PMMA ionomer blends were about 30% higher. When comparing the elongation, pure Nylon-11 were found to be similar to the Nylon-11 / PEAA ionomer blends, but the Nylon-11 / PMMA ionomer blends were found to be reduced by as much as 20%. On the other hand, the change due to the content of ionomer showed a decrease in both tensile strength and elongation as the content in the two blend systems increased. Thus, it can be concluded that the mechanical properties of nylon 11 were affected more strongly by the type of main chain of ionomer rather than the ionomer contents.

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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

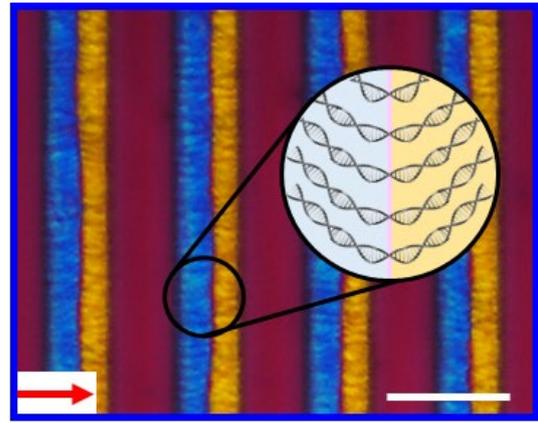
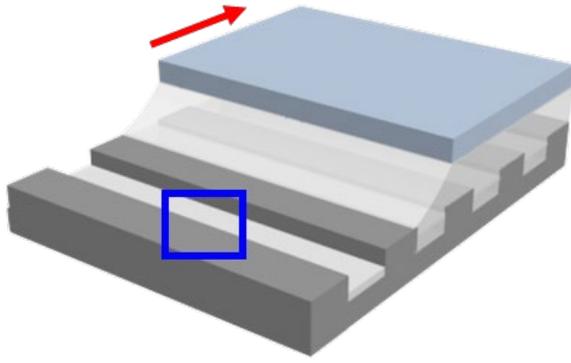
Fabrication of two-dimensional DNA microstructures via topographic control and shear force

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*

Controlling the orientation of DNA molecules is quite difficult due to the long contour length and flexibility but positively necessary for utilizing DNA as a building block and forming the micro- or nanostructures. DNA, one of the biopolymers, has recently emerged as a promising building block because it is sustainable in nature, shows liquid crystal phase depending on the concentration, and can be functionalized by electrostatic interaction. Therefore, we developed a technique to control the orientation of DNA chains in a thin film by using shear-induced pre-alignment and bulk elastic properties of the DNA liquid crystal phase. The technology can easily control the orientation of DNA in a large area but for designing the nanostructure with high integration and using applications such as organic electronics, inorganic particle array, and other lithographic templates, patterning at a microscopic scale is also required. To fabricate complicated two-dimensional micro- or nanostructures of this soft material, predesigned substrates can be applied for confinement. Then, a unique and complex structure can be formed spontaneously due to the interaction between the elastic properties of DNA and the confinement effect of the substrate. Here, we conducted the pulling experiments on square-lattice micro-channel substrates to form novel and sophisticated DNA nanostructures. Alphabet 'U'-like morphology is generated and the pattern of the DNA in the valley of the channel can be modulated by channel width. This will help to understand the self-assembly of DNA molecules in confined geometry and can provide applications to bio-template for polymers, liquid crystals or other nanoparticles.



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

Polymer Chemistry

Zoom 1 FRI 15:00~16:00

Effect of polar and non-polar plasticizers on the mechanical properties of poly(styrene-co-methacrylate) ionomers of various ion concentrations

In-Hwa Choi, Joon-Seop Kim^{1,*}

department of advanced materials engineering, Chosun University, Korea

¹*Department of Polymer Science and Engineering, Chosun University, Korea*

Ionomers are composed of a matrix region with few ionic groups and a cluster region with many ionic groups. In this study, we investigated the polar (Glycerol) and non-polar (Dioctyl phthalate; DOP) plasticizer effects of the mechanical properties of 6.4 mol% ionomers with similar size matrix and cluster regions and 22.4 mol% ionomers composed only of cluster regions. The results show that for a 6.4 mol% ionomer, Glycerol has little matrix peak change and the cluster region is disrupted, but DOP decreases linearly in both matrix and cluster peak. For 22.4 mol% ionomers configured only on a single cluster, both Glycerol and DOP cluster peaks are significantly reduced. Polystyrene composed only on matrix has almost no peak change in Glycerol, and DOP decreases linearly. This tells us that DOP is a common plasticizer that affects matrix and multiplet, while Glycerol is a plasticizer that only affects multiplet.

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

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Dynamic mechanical properties of PLA and random poly(styrene-co-methacrylate) ionomer blends

Sang Hui Park, Joon-Seop Kim^{1,*}

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¹Department of Polymer Science and Engineering, Chosun University, Korea

In this study, the mechanical properties of poly(styrene-co-methacrylate) ionomer blends neutralized with PLA, Na(I) and Li(I) were studied. The glass transition temperature (T_g) of PLA was about 70 °C, and the T_g of ionomer was 150 °C and 250 °C. On the other hand, only one T_g was shown between 115–125 °C for the PLA-Na ionomer blend and 125–145 °C for the PLA-Li ionomer blend. These results indicated that both ionomers could increase the T_g of PLA by more than 40 °C. And in the case of storage modulus at temperatures above T_g , PLA flowed. However, for each ionomer blend, the rubbery modulus gradually increased in the range of 10^5 – 10^6 as the ionomer content increased to 30-70 wt%. Therefore, in this experiment, it was found that the ionomer neutralized with Na⁺ and Li⁺ was helpful in improving the thermal properties of PLA.

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

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Biodegradable Mesoporous Organosilica Nanoparticle Drug Delivery Platform with Dual-targeting Protein affibody

Gyeongseok Yang, Ja-Hyoung Ryu*

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

The usage of Protein Corona Shielded Nanoparticles (PCSNs) as a nanocarrier is effective targeting way of the drug delivery system. It is attaching functionalized protein onto the Mesoporous silica nanoparticles (MSNs) in advance, and functional protein inhibits protein adsorption which induces phagocytosis by macrophage. However, the investigation of controlled drug release profile of PCSN inside the cancer cell is still challenging for the perfection of the drug delivery. Because protein corona may inhibit the drug release from the nanoparticle. Although MSN could encapsulate high amount of hydrophobic drug, due to their property of staying inside nanoparticles may inhibit the drug release, it is needed to facilitate the drug release from inside of the nanoparticle. To give PCSN a function of the controlled release, the stimuli-responsive, and Biodegradable Mesoporous Organosilica Nanoparticles (MONs) could be better strategy in aspects of controlled release. MONs are consisted with silica containing disulfide bond, which response with higher GSH concentration of the tumor micro environment. The disulfide bond of MONs can be reduced by the GSH and degraded achieving better release than the conventional Mesoporous Silica Nanoparticles (MSNs). This degradation can occur higher amount of the delivery of the drug, leading to the effective cancer cell death than the MSNs. Not only enhancing the release profiles, it is expected to achieve universality of the protein modification, with various kinds of the protein-affibody. Dual modification can induce the enhanced effect of the targeting cancer cells, giving universality to the nanocarrier.

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

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Study of catechol-modified chitosan 3d printing of porous structure.

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Department of Chemistry, Sejong University, Korea

¹*chemistry, Sejong University, Korea*

Catechol-substituted chitosan (CCS) was synthesized by introducing a catechol group into natural chitosan, and a chitosan gel was formed by using a coordination bond between the catechol group and Fe ions, from which a porous material was developed. It was confirmed by gel formation and Raman spectroscopy that the catechol group and Fe ions of CCS form a coordination bond. To increase the mechanical strength, high molecular weight chitosan (CS) was selected, a CCS/CS mixed solution was prepared at various molar ratios, and the solution cast by a doctor blade was immersed in an aqueous Fe ion solution to prepare a porous material through phase inversion. The morphology of the porous material obtained according to the CCS/CS molar ratio and solid phase concentration was confirmed by SEM, the porosity was measured, and the correlation was investigated. It is confirming its applicability as a gel printing material for the development of a new biocompatible CCS/CS porous material with a three-dimensional structure.

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

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Synthesis of Mesoporous Polymer Membranes with Tailored Surface Charges

Taeseok Oh, Myungeun Seo*

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

Mesoporous polymer membranes possessing well-defined and interconnected mesopores can be an attractive option as membranes in electrochemical devices by offering permselectivity based on the pore size and surface charges. Here we explore the synthesis of mesoporous polymer composites carrying positive and negative charges on the pore surface. We employ polymerization-induced microphase separation in the presence of macroporous support to produce a cross-linked and reinforced block polymer membrane in one step, that can be readily converted into mesoporous by selective etching. Different charges are introduced on the surface by postfunctionalization reactions with control over charge densities. Detailed synthetic routes and characterization of the resulting membranes will be presented.

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

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Crystallization of 1-dimensional hypo-crystal polycarbonate by rapid thermal quenching

Thanh Van Vu, Youngjong Kang*

Department of Chemistry, Hanyang University, Korea

Poly (bisphenol-A carbonate) (PC) is an intrinsically crystallizable polymer that numerous crystallization methods were reported, however, most of them provided spherulite crystal structure. Recently, 1-dimensional crystallization concept of stereo-irregular *atactic*-PMMA with strong mechanical property by using entropy diluent was reported. Hypo-crystalline PC (hc-PC) was similarly prepared by rapid thermal quenching process using benzoic acid (BA) as entropy diluent. Also, for comparison, some conventional crystallizations of PC were performed. While 3D orthorhombic structure was obtained in other crystallization methods, hc-PC exhibited 1-D fiber-like structure with ordered lateral packing between chains (d -spacing = 4.1 and 3.4Å) which is independent from chain conformation and the other two dimension was still amorphous. Due to a different conformation conversion during crystallization, 1-D hc-PC provided different thermal property that originally shows clear melting transition at 225°C but could be shifted to 285°C by thermal annealing.

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

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Development of hydrogel-based lateral flow diagnostic device

Nayoon Pyun, Kwanwoo Shin^{1,*}

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Point-of-care devices that enable quick diagnosis in the field are very important in the diagnosis of infectious diseases that have recently emerged as a major problem worldwide and in poor medical environments such as developing countries. Paper-based lateral flow strip using capillary phenomenon is in the spotlight because it is easy to manufacture and use, cost-effective, and does not require experts. Cellulose, a material familiar to us as the major constituent of paper, is mainly used for the production of conventional strip. But it is chemically inert to immobilize the biomolecule that need to catches the analyte, and it is difficult to control the flow rate. In this research, we introduced hydrogel which is formed by chemically cross-linking of the various monomers into the strip to manufacture new concept of lateral flow kit. We can control the pore size and affinity for biomolecules through the composition and concentration of the various monomer, as well as increase the sensitivity by controlling the flow rate.

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

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Development of high dielectric material using polyimide/metal nanocomposite

Jun Woo Park, Jeongdong Kim, 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, as the market for electronic devices such as smart phones and tablet PCs expands, research on energy storage devices applied to miniaturized and light-weight devices is being conducted, and capacitors are attracting attention as miniaturized electronic devices. Although ceramic is used as a major material for capacitors, it has limitations such as environmental issues related to manufacturing, increased raw material prices, area occupied by devices, and limitations in miniaturization. Herein, we report the synthesis of PI/Cu nanoparticles as a high dielectric composite filler for polymer-matrix composites(PMC) that can be used as an embedded capacitor by using polyimide and copper precursor. Polyimide is a high heat-resistant engineering plastic material with high thermal stability, chemical resistance, and insulation properties. PI/Cu nanoparticles can improve dispersion in solvents, and use polystyrene together as a matrix material to have a dielectric constant of 320 and a dielectric loss value of 0.04, as well as a leakage density of 200 nA/cm². It enables application as a filler material of high dielectric composites.

Poster Presentation : **POLY.P-29**

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

EFFECT OF DIOLS STRUCTURE TO GLYCOLYSIS OF D-ISOSORBIDE-CONTAINING COPOLYESTERS

Minh Dieu Ngo, Kyuwon Sim, 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*

D-Isosorbide (ISB), an attractive diol biologically originated from starch, has appeared as a potential candidate for copolymer manufacture due to its enticing properties. However, containing a complex structure hampers hydroxyl groups in ISB from participating in glycolysis reaction resulting in an obstacle to the recycling of ISB copolymers. In this study, bis(6-hydroxyhexahydrofuro[3,2-b]furan-3-yl) terephthalate (BHDIT), a monomer of poly(isosorbide terephthalate) (PIT), was synthesized and carried out under transesterification reaction to investigate the effect of steric hindrance of bicyclic structure and secondary alcohol. In comparison with poly(ethylene terephthalate) (PET) and poly(cyclohexylendimethylene terephthalate) (PCT), PIT displayed a considerably high stability in the glycolysis of PET-PCT-PIT copolyesters. Besides, the glycolysis of PET with ISB resulted in a dramatically reduced reaction rate, which was less than 0.2% of that with diethylene glycol.

Poster Presentation : **POLY.P-30**

Polymer Chemistry

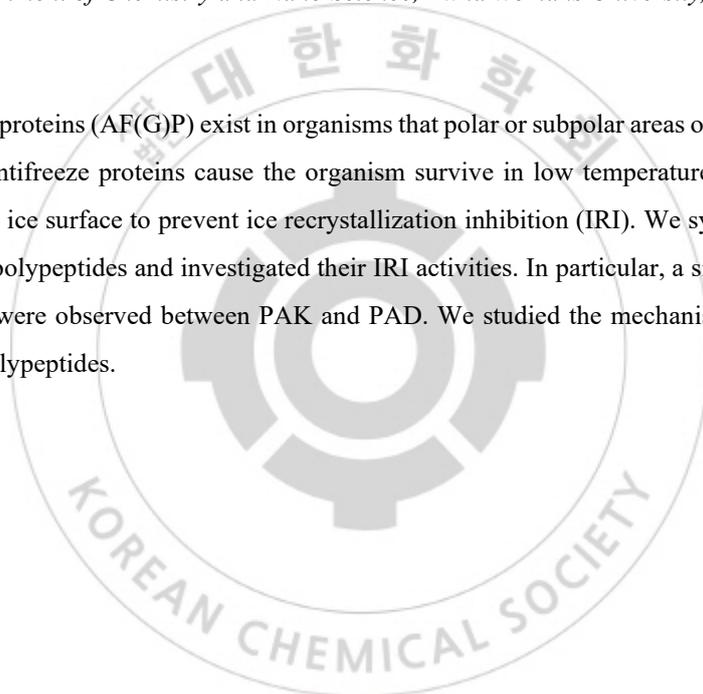
Zoom 1 FRI 16:00~17:00

Ice recrystallization inhibition activity of synthetic polypeptides

Zhengyu Piao, Byeongmoon Jeong^{*}, Hyun Jung Lee

Department of Chemistry and Nano Science, 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 low temperature environments. This protein binds to the ice surface to prevent ice recrystallization inhibition (IRI). We synthesized a series of AFGP-mimicking polypeptides and investigated their IRI activities. In particular, a significant differences in the IRI activity were observed between PAK and PAD. We studied the mechanistic difference in IRI between the two polypeptides.



Poster Presentation : **POLY.P-31**

Polymer Chemistry

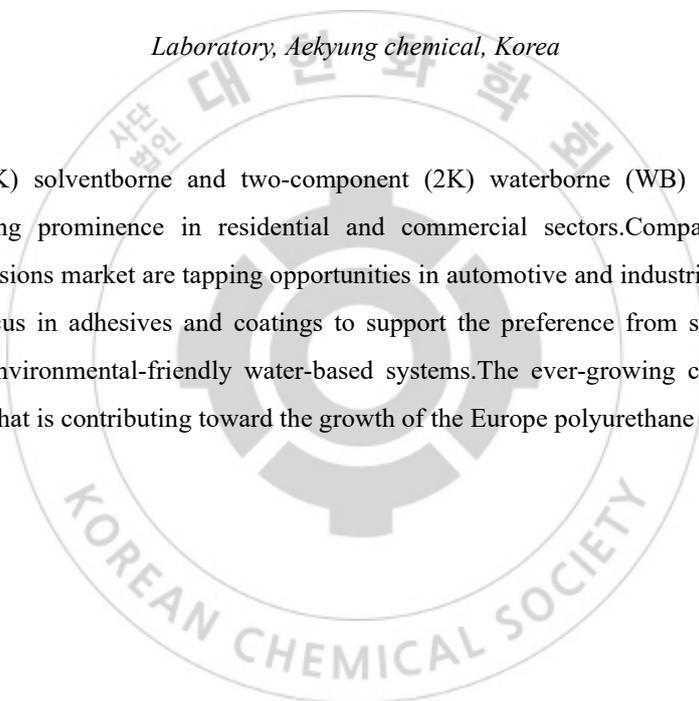
Zoom 1 FRI 16:00~17:00

Secondary dispersion acrylic polyol for high-performance waterborne coating

Seung Hyun Park

Laboratory, Aekyung chemical, Korea

one-component (1K) solventborne and two-component (2K) waterborne (WB) polyurethane (PUR) coatings are gaining prominence in residential and commercial sectors. Companies in the Europe polyurethane dispersions market are tapping opportunities in automotive and industrial coatings. They are increasing their focus in adhesives and coatings to support the preference from solvent-based coating systems to more environmental-friendly water-based systems. The ever-growing construction sector is another key driver that is contributing toward the growth of the Europe polyurethane dispersions market.



Poster Presentation : **POLY.P-32**

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Formulation of Nanocomposite Hydrogel for 4D Printed Heat Responsive Waterless Soft Actuator

Monica cahyaning Ratri, Jungju Ryu¹, Kwanwoo Shin^{2,*}

chemistry, Sogang University, Indonesia

¹*Department of Chemistry, Hanyang University, Korea*

²*Department of Chemistry, Sogang University, Korea*

Soft actuator, bio-inspired mimicking system is the one of strategy in the medical, soft robotic, pharmaceutical, and tissue engineering due to its dynamic movement toward the presence of external stimuli. By enhancing the additive manufacturing technique and material synthesis, a 4D printing system can be generated through this process. The 3D printed object offers sophisticated and innovative functions such as jumping, complex 3D movement, gripping and releasing. Combination of different formulation of ink, such as active and passive material, can be harnessed to initiate the soft actuator movement expectedly. Poly (N-isopropyl acrylamide) (PNIPAAm) is one of the well-known as active polymers that has temperature sensitive property, shrinking above the lower critical solution temperature (LCST) and swelling below LCST. As a passive material Poly-acrylamide (AAm) combined with alginate has high toughness and elasticity. Due to its surface plasmon resonances (SPR) properties, gold nanorods can absorb light, and release heat to its surrounding. Therefore, the illumination on the nanoparticle with Near Infrared (NIR) can generate heat locally and initiate the heat-induced actuation to PNIPAAm containing matrices. The irradiation of the NIR lamp had done outside the water, the waterless actuating process is one of the advantages of this system. We formulated and tested PNIPAAm-metal nanoparticle composites as an ink material to fabricate the heat-sensitive soft actuators for photo-responsive soft robotic motions. In this study, the printability and mechanical properties of the nano-composite bio-ink tested by mechanical measurements, and photo-induced heat responsiveness. We will present our preliminary results how we can formulate the nanocomposite ink, and heat-responsive reactions of the 3D printed soft actuators. Keywords: Gold nanorods, 4D printing, Waterless soft actuator, PNIPAAm

Poster Presentation : **POLY.P-33**

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Catalase Conjugated Metal-Organic-Framework for Effective Photodynamic Therapy by Relieving Tumor Hypoxia

Youjung Sim, Huyeon Choi, Myoung Soo Lah^{1,*}, Ja-Hyoung Ryu^{1,*}

Ulsan National Institute of Science and Technology, Korea

¹Department 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 : **POLY.P-34**

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Multivalent Interaction using Polymerization-induced Self-Assembly inside Mitochondria for Anti-Cancer Treatment

Sangpil Kim, Ja-Hyoung Ryu^{1,*}

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

The intracellular biomacromolecules including proteins, DNA, and polysaccharides, play an important role to perform cellular function. These macromolecules are synthesized by the polymerization of small molecules such as amino acids, nucleotides, and monosaccharides, but they have distinct properties that the small molecules do not have. For example, the amino acid itself has no enzymatic activities and trivial interactions with proteins. Proteins which has well-ordered 3D or 4D structure, however, can perform various enzymatic activities and involve important cellular signaling by multivalent interaction. By mimicking the natural system, we found that polymerization of building block give a great platform to form assembled structure for multivalent interaction with bio-macromolecules. Thus, we developed polymerization induced self aseembly of KLAK sequence to bind with mitochondrial membrane via multivalent interaction for inducing dysfunction of mitochondria, leading to apoptosis of cancer cells specifically. This polymerization shows great potential for anticancer treatment against various cancer cell lines, including drug-resistant cancer cells

Poster Presentation : **POLY.P-35**

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Synthesis of Water Repellency Composite Coating Based on Fluorosilicone Resin

Jong-tak Lee, Jae Young Bae*

Department of Chemistry, Keimyung University, Korea

A silicone resin having water repellency was synthesized by polymerizing a fluorosilane monomer. The fluorosilicone resin was synthesized to enable curing by introducing a methacrylic functional group, and the synthesized resin was analyzed through Si-NMR, GPC, and FT-IR. The synthetic resin was coated on the glass and cured by a thermal curing method. The water-repellent performance of the coated glass was confirmed by measuring the water contact angle, and the water contact angle tended to improve as the fluorine content increased. However, as the fluorine content increased, the methacrylic functional group decreased and the curing time tended to increase, which is explained that the proper content between the two functional groups became an important factor.

Poster Presentation : **POLY.P-36**

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Internal structures of polymer networks crosslinked by catechol mediated reactions

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¹*Department of Chemistry, Hanyang University, Korea*

This study explores the internal structures of catechol-functionalized polymer networks with different types of Fe³⁺-induced crosslinking. Catechol groups induce the two main reactions of covalent catechol-coupling and Fe³⁺-catechol coordination bonds. Here, we reveal the structural changes governed by the crosslinking types. First, we compared the non-ionic polymer networks (4-arm polyethylene glycol: 4PEG) with polyelectrolyte (hyaluronic acid). Second, we probed the structure crosslinked with different types of catechol mediated bonds of 4PEG chains which were modified with catechol moieties at the end groups. Catechol groups develop the various network structures in presence of Fe³⁺ ions, allowing covalent bonds and coordination bonds of mono, bis, and tris complexes under the pH controls. We investigated the internal structures of networks by using X-ray scattering measurements. The results revealed the chain conformation dominantly influences the network structure for polyelectrolyte. On the contrary, the structures of non-ionic polymers were demonstrated by the linkages based on the crosslinking types. The observations here suggest that various structural characteristics can be considered to revive abundant applications using biopolymers.

Poster Presentation : **POLY.P-37**

Polymer Chemistry

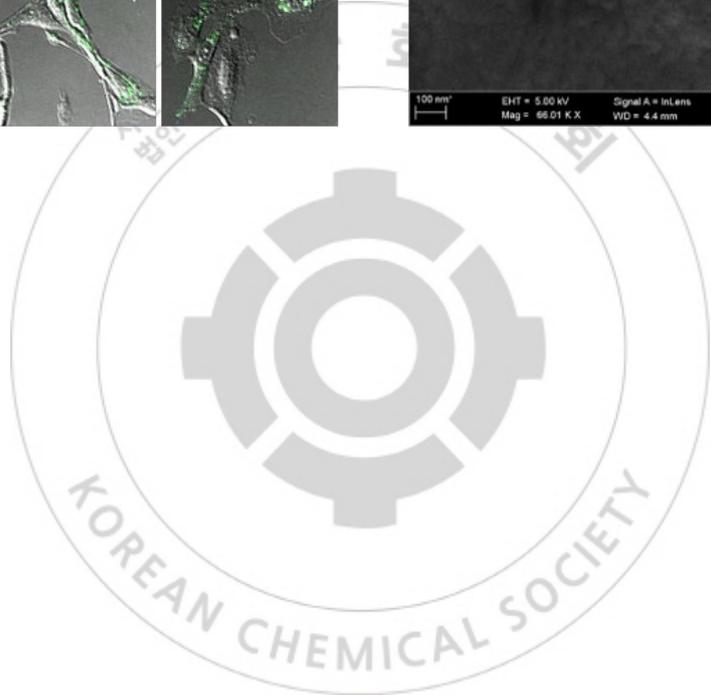
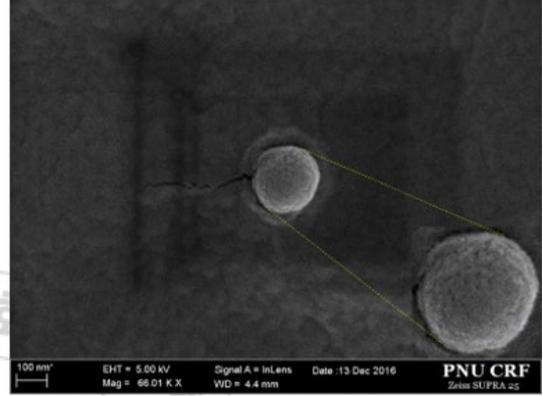
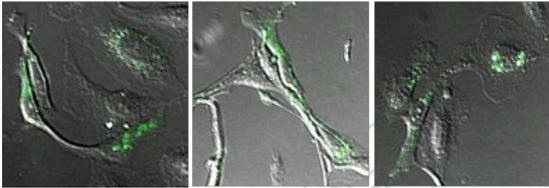
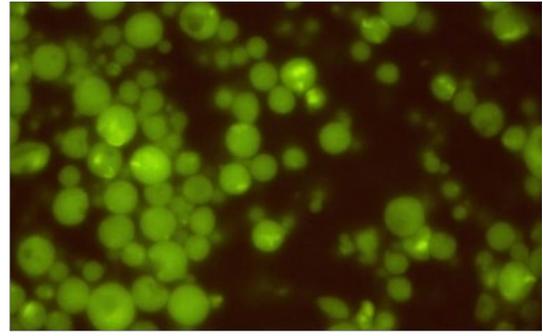
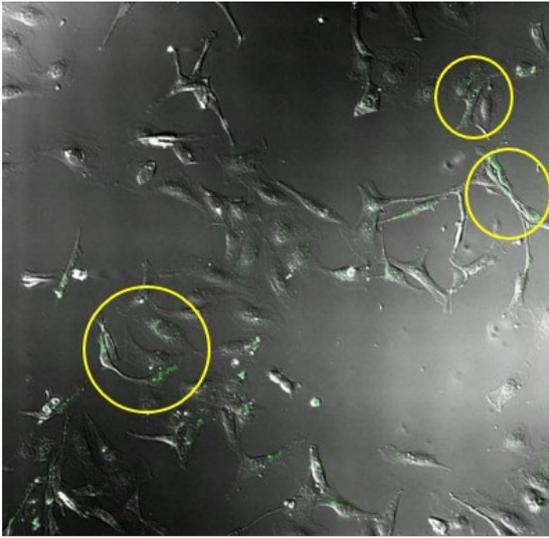
Zoom 1 FRI 16:00~17:00

Gene / drug delivery studies based on synthesized biodegradable LTU and PFU nanoparticles

Soo-Yong Park, Ildoo Chung*

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

Gene therapy is a good alternative to drugs in chemotherapy due to drug resistance and toxicity and known to lower the occurrence probability of mutation of cells through gene carrier. Herein, gene carrier nanoparticles with minimal toxicity and high transfection efficiency were fabricated from biodegradable polymer (L-tyrosine polyurethane, LTU), which was pre-synthesized from desaminotyrosyl tyrosine hexyl ester (DTH), and polyethylene glycol (PEG) and used to evaluate their potential biological activities molecular controlled release and transfection studies. 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 the drug or gene, to avoid the immune system their surface was modified with PEG.



Poster Presentation : **POLY.P-38**

Polymer Chemistry

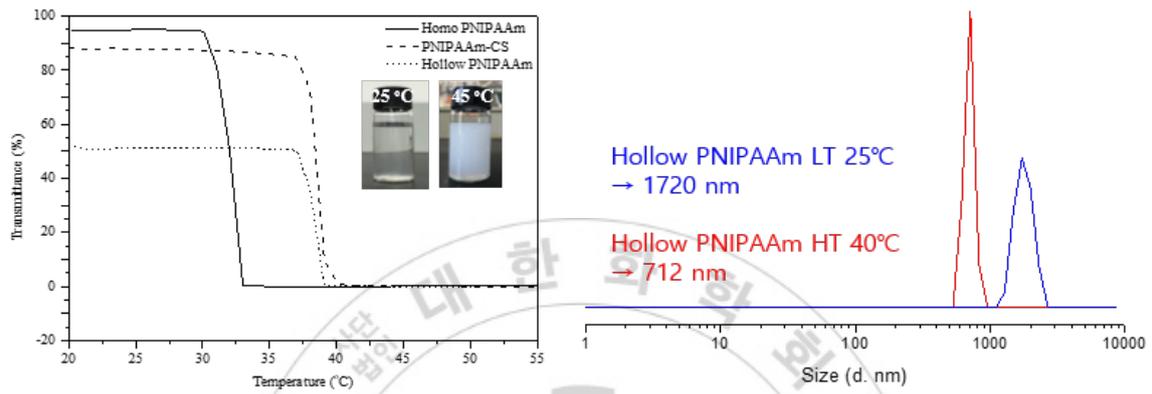
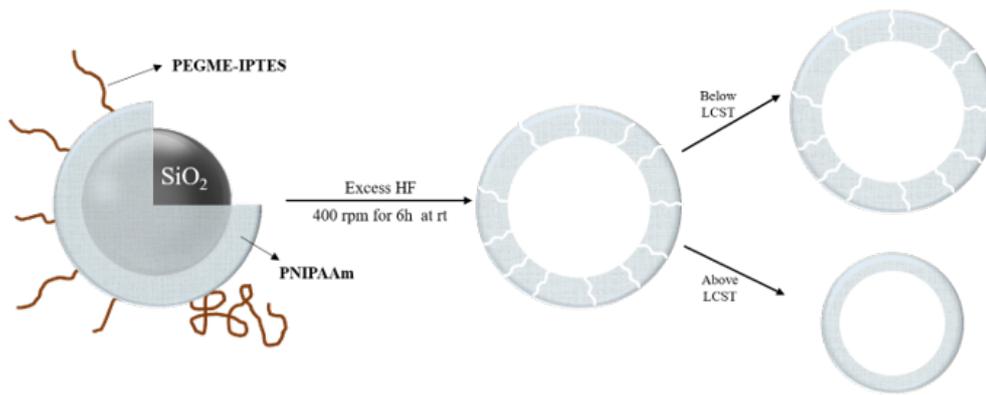
Zoom 1 FRI 16:00~17:00

Study on the thermoresponsive hollow-shell polymeric capsule based on colloidal silica

Soo-Yong Park, Ildoo Chung*

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

In this study, thermoresponsive polymeric hollow-shell nanoparticles with a hole connecting the outside with the inside were synthesized from colloidal silica (CS) and 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 (NH₃) 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. The nanoparticles were prepared by modified silica with 3-(trimethoxysilyl) propyl methacrylate (MPS) and PEGME-IPTES by the polymerization of poly(N-isopropylacrylamide) (PNIPAAm), then the silica core and PEGME-IPTES chain were removed by etching with hydrofluoric acid. Thermoresponsive polymeric hollow nanoparticles were characterized by ¹H NMR, ¹³C NMR, UV-vis and FT-IR spectroscopies. The particle size distribution was also determined with DLS, TEM images.



Poster Presentation : **POLY.P-39**

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

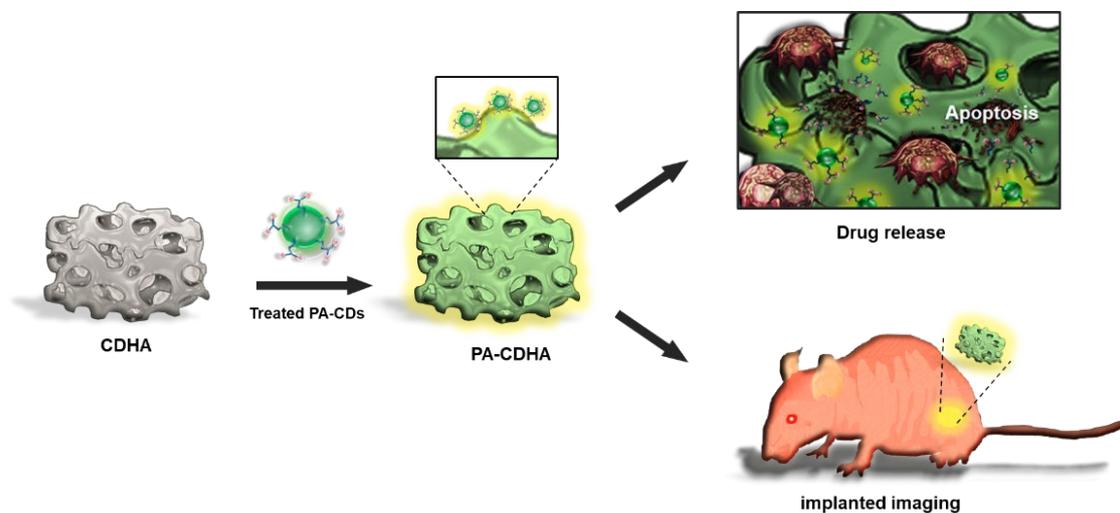
Alendronate-Conjugated Carbon Dots for Osteoclasts Inhibition and Implanted Fluorescence Imaging

KyungKwan Lee, Chang-Soo Lee^{1,*}

*Hazards Monitoring Bionano Research Center, Korea Research Institute of Bioscience & Biotechno,
Korea*

¹*BioNanotechnology Research Center, Korea Research Institute of Bioscience & Biotechnology, Korea*

Bone graft using biomaterials have attracted a great deal of interest in the past years. As a primary bioceramic material for bone graft, calcium phosphate is one of best biomaterial for reconstruction of bone disorders. Herein, we describe the fabrication of phytic acid-alendronate conjugated carbon dots (PA-CDs), which applicable to calcium-based bioceramics to impart functionality of bone graft material. The capability of PA-CDs functionalized calcium-deficiency hydroxyapatite (CDHA), termed as PA-CDHA, not only possess the capability of biocompatibility, but also have offered attractive opportunity for both in vivo implanted fluorescence imaging and osteoclasts suppression by alendronate release. These outstanding results have indicate that it is possess theranostics capability and applicable to the field of bone graft materials.



Poster Presentation : **POLY.P-40**

Polymer Chemistry

Zoom 1 FRI 16:00~17:00

Synthesis and Characterization of Organic Light-Emitting Diodes (OLEDs) Materials

Na Young Goo, Yun Hi Kim^{1,*}

Chemistry, Gyeongsang National University, Korea

¹Department of Chemistry, Gyeongsang National University, Korea

In this study we studied OLEDs materials. In general, OLEDs can be classified into 1st, 2nd, and 3rd generation. First-generation OLEDs use a fluorescent method and have a disadvantage of inferior efficiency. Second-generation OLEDs have 100% internal quantum efficiency, but they have a disadvantage in terms of cost because they use transition metal compounds such as iridium and platinum. To compensate for the shortcomings, the 3rd generation OLEDs using TADF material can represent 100% internal quantum efficiency by fluorescence. However, TADF materials causes a problem that the half-width of the EL spectrum is broad and the color purity of the OLEDs light-emitting element is deteriorated. Therefore, Solving these problems is very important in OLEDs material development. In this work, we developed new TADF blue emitting material. The synthesis and characterization of new TADF blue emitting material will be discussed.

Poster Presentation : **POLY.P-41**

Polymer Chemistry

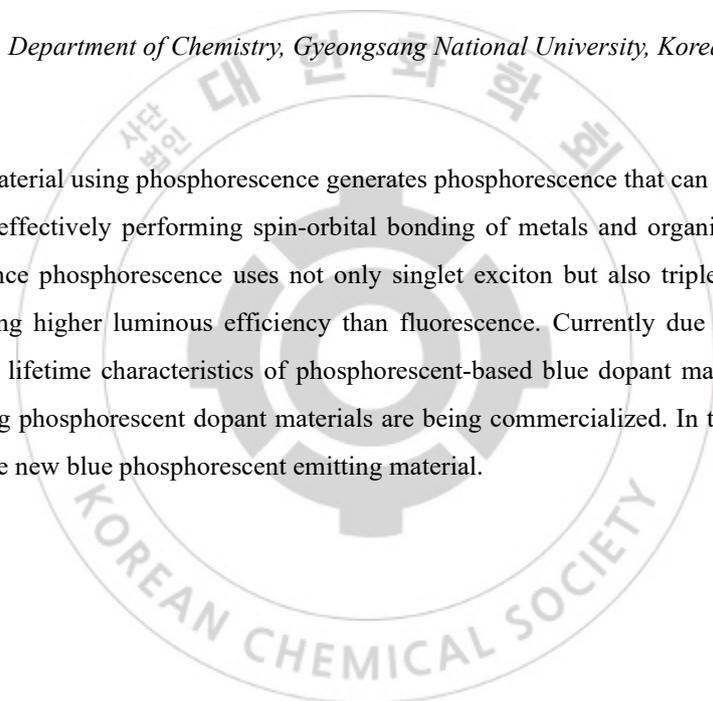
Zoom 1 FRI 16:00~17:00

Synthesis and Characterization of Blue Phosphorescent Emitting Material

Ji Hyun Lee, Yun Hi Kim*

Department of Chemistry, Gyeongsang National University, Korea

A light-emitting material using phosphorescence generates phosphorescence that can have high-efficiency characteristics by effectively performing spin-orbital bonding of metals and organics due to the heavy element effect. Since phosphorescence uses not only singlet exciton but also triplet exciton, it has the advantage of having higher luminous efficiency than fluorescence. Currently due to insufficient color characteristics and lifetime characteristics of phosphorescent-based blue dopant materials, only red and green light emitting phosphorescent dopant materials are being commercialized. In this study, we design and synthesis of the new blue phosphorescent emitting material.



Poster Presentation : **POLY.P-42**

Polymer Chemistry

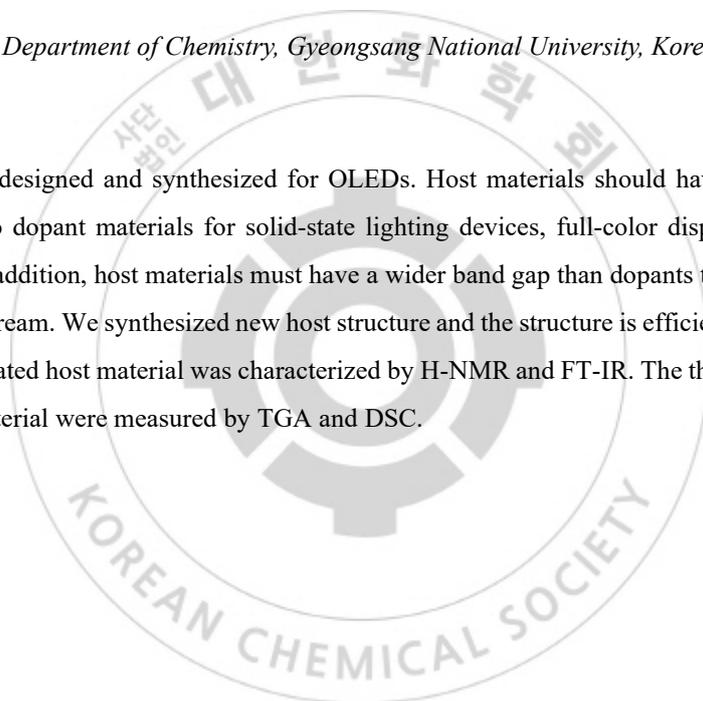
Zoom 1 FRI 16:00~17:00

Synthesis and Characterization of New Host Material for Organic Light Emitting Diodes (OLEDs)

Ji Eun Lee, Yun Hi Kim*

Department of Chemistry, Gyeongsang National University, Korea

A host material is designed and synthesized for OLEDs. Host materials should have a efficient energy transfer function to dopant materials for solid-state lighting devices, full-color displays and stability at affordable cost. In addition, host materials must have a wider band gap than dopants to prevent electron of dopant from backstream. We synthesized new host structure and the structure is efficient. The structure and properties of fabricated host material was characterized by H-NMR and FT-IR. The thermal characteristics of the designed material were measured by TGA and DSC.



Poster Presentation : **POLY.P-43**

Polymer Chemistry

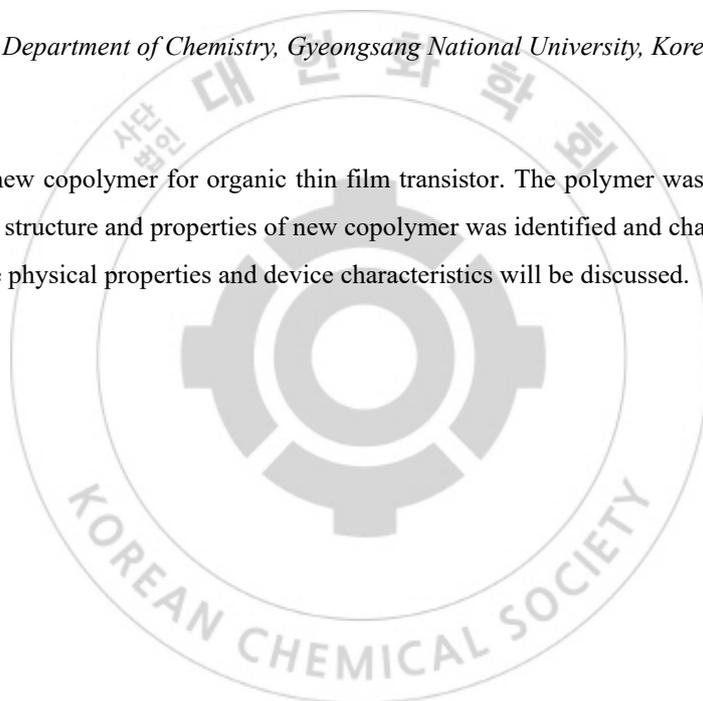
Zoom 2 FRI 15:00~16:00

Synthesis and Characterization of New Copolymer for Organic Thin Film Transistor (OTFT)

Jihyun Park, Yun Hi Kim*

Department of Chemistry, Gyeongsang National University, Korea

We synthesized a new copolymer for organic thin film transistor. The polymer was synthesized through stille coupling. The structure and properties of new copolymer was identified and characterized by various spectroscopies. The physical properties and device characteristics will be discussed.



Poster Presentation : **POLY.P-44**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

SYNTHESIS AND CHARACTERIZATION OF NEW ACCEPTOR FOR OPV

Seung Hun Lee, Yun Hi Kim^{1,*}

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¹*Department of Chemistry, Gyeongsang National University, Korea*

This is the content of the non-fullerene single molecule acceptor material for organic solar cells. Fullerene derivatives, which have been widely studied as electron acceptors in the field of organic solar cells, have high conductivity, but have difficulty in commercialization such as low oxidation stability and high unit cost. In addition, there are various limitations such as low absorbance in the visible light region and difficulty in purification and synthesis. Recently, for the commercialization of organic solar cells, many new electron acceptor materials that can replace high-efficiency and low-cost fullerene structures have been developed. In this study, a new acceptor-donor-acceptor type acceptor molecule with DTBBDT was synthesized and analyzed. DTBBDT is expected to have high hole mobility due to good packing between molecules by imparting flatness to the backbone. In addition, it is expected that higher light conversion efficiency will be obtained when BHJ is formed with the donor material by increasing the solubility by introducing an alkyl chain substituent in the side chain.

Poster Presentation : **POLY.P-45**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Comparison of Transesterification reaction Efficiency with Catalysts in Polymer Solution and Vitrimer

Changjun Oh, Youngjong Kang*

Department of Chemistry, Hanyang University, Korea

General thermosetting polymers have better physical properties than thermoplastic polymers, but are difficult to recycle. A recent study reported a thermoset polymer called vitrimer that can be recycled using a variety of dynamic covalent bonds. Vitrimer has a temperature called topology freezing transition-temperature(T_v) at which the bond exchange is activated. Vitrimer can be reshaped above T_v . Activation of transesterification is known to be possible only at high temperatures. Selecting the appropriate catalyst for reshaping at lower temperatures is necessary. However, it is difficult to compare the catalyst directly with the vitrimer. We compared the catalyst's efficiency relatively easily through a simple polymer solution system. We present new possibilities in controlling the operating temperature of vitrimer through this study.

Poster Presentation : **POLY.P-46**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Optimization of synthesis process 2D material MXene: Manganese carbide – New material of MXene group

Ngoc Bao Tran, Youngjong Kang^{1,*}

Chemistry Department, Hanyang University, Korea

¹*Department of Chemistry, Hanyang University, Korea*

MXenes (two-dimensional transition metal carbide, carbonitrides and nitrides) was first discovered in 2011, there are several compositions belong to this new 2D group that has been synthesized. In recent years, the publications about MXenes were more and more increasing due to their properties such as high electrical conductivity, functional terminal surface, which can be applied in immersion application (the most well-known is energy storage, and water purification, electromagnetic interference shielding) as well as their unknown theoretically. From MAX phase, the etching process can remove the metal layers to obtain the MXene structure. Our research stays focus to use the MXene of Manganese metal by using sodium fluoride and hydrochloric acid as etching solution (instead of hydrofluoric acid), we first use Mn₂AlC as the precursor and synthesis Mn₂CT_x, at first we will investigate the affection of the temperature, time and also concentration of etching solution.

Poster Presentation : **POLY.P-47**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Sequence-Controlled Synthesis of Core-Crosslinked Star Polymers via Single Chain Collapse

Jiyun Nam, Jae suk Lee¹, YongJoo Kim², 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*

Core-crosslinked star (CCS) polymers represent globular nanoparticles where linear polymeric arms radiate from the cross-linked core. An arm-first method has been generally employed for the synthesis of heteroarm CCS polymers by copolymerization of different macromonomers with a cross-linker such as divinylbenzene. However, control of arm number and compartmentalization with distinct arms has been challenging. Here, we introduce a new synthetic approach to CCS polymers by single chain collapse of well-defined graft copolymer precursors. We prepare sequence-controlled graft copolymers via grafting-through copolymerization and collapse them by intramolecular dimerization. Synthesis, characterization, and self-assembly behavior of the CCS polymers will be discussed.

Poster Presentation : **POLY.P-48**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

In-situ Fabrication of Vitrimer-Carbon Nanotube Composite via Solventless Mechanochemical Approach

Wansu Cho, Chiyong Park*

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

Vitrimer, a new class of material which shows linear viscosity changes upon heating like vitreous silica through dynamic covalent bond networks, has features of thermoplastic and thermoset at the same time. Owing to this advantage, it has been attracted lots of intentions as a promising material for polymer composite with multi-functional properties. Unfortunately, formation of such polymer composites requires a long period of dispersing and drying process due to using toxic solvents for uniform dispersion of additives and homogeneous chemical reaction of polymer. Herein, we suggest a eco-friendly and in-situ process to form vitrimer-CNT composites via solventless mechanochemical approach.

Poster Presentation : **POLY.P-49**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Green chemical one-pot synthesis of cationic cellulose nanocrystals

Bon-Jun Ku, Chiyong Park*

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

Ionic liquid assisted process enabled one-pot synthesis of pyridinium salt cellulose nanocrystals using methylimidazolium chloride ionic liquid. The reaction consists of grafting (esterification and a nucleophilic attack on the C–Br bond by pyridine) and dissolution of cellulose (hydrogen bond breakage of cellulose by ionic liquid). This reaction leads to nanoization and functionalization of cellulose at once. The surface substitution ratio of the pyridinium salt on the resulting cellulose nanocrystals was demonstrated through XPS, zeta potential, and dye adsorption analysis. Cationization of cellulose nanocrystals could further open up other innovative applications such as gene and drug delivery, vaccine adjuvants, and tissue engineering. This simple process, use of little organic solvent and reusability of ionic liquid are expected to be used as a meaningful reaction path from an environmentally, but also economically.

Poster Presentation : **POLY.P-50**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Multi-Responsive Nanocapsules and Gel Composites Tailored with Metal-Phenolic Network

Gyeonghyeon Choi, Chiyoung Park*

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

Porous nanoparticles with responsive molecular valves that show drug release in response to various stimuli such as pH, light, redox, enzyme have great interest for use in molecular robotics and biomedical applications. Those molecular valves are ideal for application in controlled release systems, but they have complicated synthesis procedures. Here, we report facile method for synthesizing multi-responsive nanocapsules and gel composites through metal-phenolic molecular valves. These valves not only efficiently entrapped guest molecules without sustain release but also confirmed pulsatile release of guest molecules under ultrasound and electrical input due to robust metal-phenolic network. Furthermore, we fabricated multi-responsive gel composites using combination of polymer matrix with nanocapsules.

Poster Presentation : **POLY.P-51**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Organocatalyzed Synthesis and Degradation of Functionalized Poly(4-Allyloxymethyl- β -Propiolactone)s

Yeji Yu, Jeung Gon Kim^{1,*}, Byeong-Su Kim^{*}

Department of Chemistry, Yonsei University, Korea

¹*Department of Chemistry, Jeonbuk National University, Korea*

Chemical synthesis of degradable poly(β -hydroxyalkanoate) (PHA) that can be produced by microorganisms allows the control of solubility, crystallinity, hydrophobicity, degradability, thermal, and mechanical properties by introducing functionality on the side chain. Herein, we synthesized a PHA derivative containing pendent allyl group via anionic ring-opening polymerization of 4-allyloxymethyl- β -propiolactone monomer with organocatalysts in bulk condition, to yield a poly(4-allyloxymethyl- β -propiolactone) (PAMPL) in a controllable manner. The prepared polymers were characterized via ¹H- and ¹³C-NMR, GPC, DSC, and MALDI-TOF/TOF. Photoactivated thiol-ene reaction allows the post-polymerization modification of PAMPLs with varying substituents. Most importantly, the PAMPL polymer the cross-linked PAMPL film are degraded by either the organocatalyst or thermal conditions.

Poster Presentation : **POLY.P-52**

Polymer Chemistry

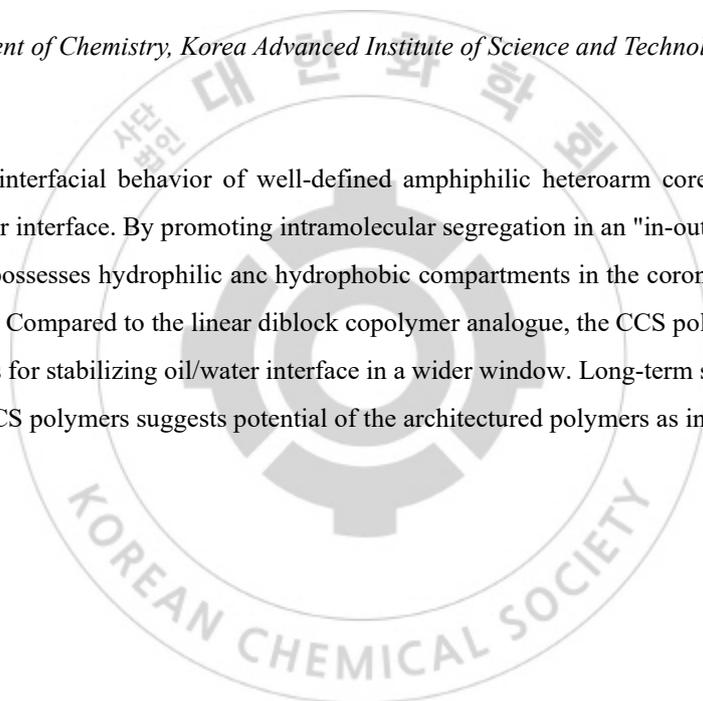
Zoom 2 FRI 15:00~16:00

Stabilization of Oil/Water interface by Core Cross-Linked Polymers as Janus Hairy Nanoobjects

Yunji Jung, Myungeun Seo*

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

Here we examine interfacial behavior of well-defined amphiphilic heteroarm core cross-linked (CCS) polymer in oil/water interface. By promoting intramolecular segregation in an "in-out" synthetic route, the resulting polymer possesses hydrophilic and hydrophobic compartments in the corona which are fixed by a cross-linked core. Compared to the linear diblock copolymer analogue, the CCS polymer shows superior interfacial activities for stabilizing oil/water interface in a wider window. Long-term stability of emulsions stabilized by the CCS polymers suggests potential of the architected polymers as interfacial agents.



Poster Presentation : **POLY.P-53**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Cooperative Hydrogen-Bonding Array of Highly Adhesive Polyethers with Carboxylic Acid Pendants

Minseong Kim, Sang Ho Lee^{1,*}, Byeong-Su Kim^{2,*}

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

¹Division of Drug Development, Korea Research Institute of Chemical Technology, Korea

²Department of Chemistry, Yonsei University, Korea

Despite successful tuning of polymer properties by intermolecular hydrogen bonding (H-bonding) between polymer chains, we envision that the further structural designs could improve by inducing dynamic interaction between inter- and intramolecular H-bonding at a single polymer chain. In this study, we introduce the design of polymer possessing both H-bond donor and acceptor moiety within a single monomer unit, allowing high level of H-bonding at the polymer chains. Specifically, we synthesized poly(glycidoxy acetate) (PGA) bearing pendent carboxylic acid groups on the polyether as a platform. The desired PGA polymer was prepared using functional epoxide monomer, tert-butyl glycidoxy acetate (*t*BGA), via monomer activated ring-opening polymerization and subsequent deprotection in a controlled manner with narrow dispersity. The prepared PGA displayed a self-association behavior in solution as well as highly adhesive bulk property owing to the combination of both inter- and intramolecular H-bonding in a polymer.

Poster Presentation : **POLY.P-54**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Antifouling Multi-Loop Copolyethers

Suebin Park, Minseong Kim¹, Byeong-Su Kim*

Department of Chemistry, Yonsei University, Korea

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

Copolymers containing poly(ethylene glycol) (PEG) has been widely used for antifouling coating materials because of its high solubility, biocompatibility, and lubrication characteristics. Unlike the polymer brush, the loop conformation has been suggested as a superior alternative for enhanced surface antifouling properties owing to its large excluded volume, and strong steric hindrance. We report herein the synthesis of antifouling multi-loop copolyethers consisting of catechol acetonide glycidyl ether (CAG) and triethylene glycol glycidyl ether (TGE) to yield poly(CAG-co-TGE)_n. Specifically, we varied the fraction of CAG monomer, a mussel inspired moiety for versatile coatings, in a fixed degree of polymerization, to study the size effect of polymeric loop in its antifouling behavior. The synthesis of the functional monomers and the anionic ring-opening polymerization together with the highly antifouling effect are discussed in the presentation.

Poster Presentation : POLY.P-55

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

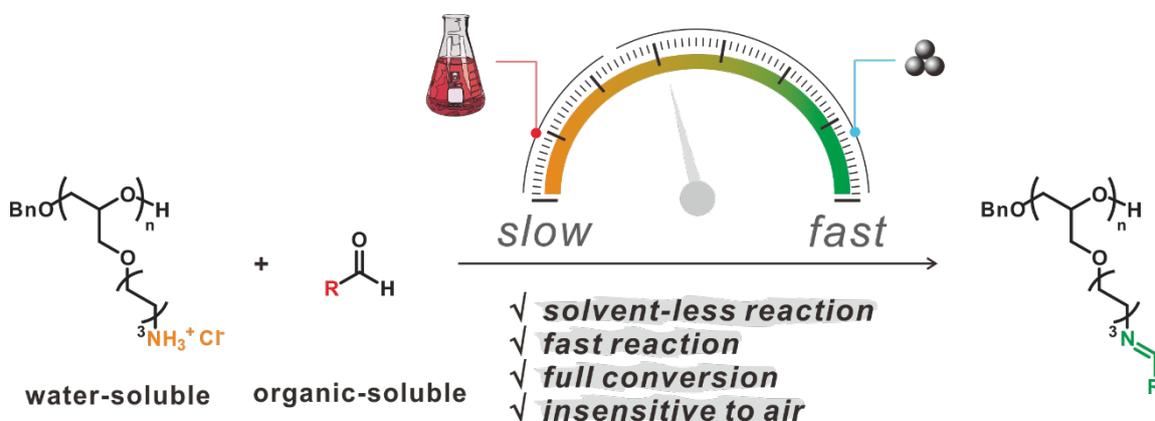
Mechanochemical Post-Polymerization Modification of Ammonium-Functionalized Polyethers

Joo Won Lee, Jeung Gon Kim^{1,*}, Byeong-Su Kim*

Department of Chemistry, Yonsei University, Korea

¹*Department of Chemistry, Jeonbuk National University, Korea*

An imine formation is generally achieved by reacting amines and aldehydes in organic solvents. However, ammonium salts are typically insoluble in organic solvents, thereby limiting conventional reaction methods. Alternatively, a solvent-free mechanochemical reaction is suggested in this study to bypass the solubility issues. Specifically, a post-polymerization modification of ammonium-functionalized polyethers is demonstrated by using vibrational ball-milling. Polyethers having ammonium pendant groups are prepared by anionic ring-opening polymerization of azidohexyl glycidyl ether followed by subsequent Staudinger reduction. The mechanochemical reaction is performed to afford the fast and efficient formation of imines in pendant groups. The versatility of a wide scope of aldehydes to this approach is evaluated and the kinetics are compared to conventional solution methods, highlighting the potentials of solvent-less mechanochemical modification of polymers.



Poster Presentation : **POLY.P-56**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Direct observation of photo-crosslinking diphenylalanine based peptides by in-situ nanoimaging

Jun Ho Hwang, Eunji Lee*

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

Peptide self-assembled nanostructures based on diphenylalanine (FF) derivatives can have an orderly beta-sheet secondary structure due to strong interactions of phenyl groups between adjacent derivatives and form nanospheres, nanocylinders, and nanotubes. In addition, its are widely applied in fields such as drug delivery and tissue regeneration due to structural stability and biocompatibility. In this study, the introduction of tyrosine amino acids involved in protein synthesis and photooxidation-reduction reaction limits the alignment of strong antiparallel structures and suggests a self-assembly control strategy to enable nanovesicle formation. This process can be confirmed through the assembly transformation behavior that occurs along with the photopolymerization, and this will be explained through an in-situ liquid cell transmission electron microscope. This indicates that in a peptide-based material design strategy, geometric limitations play an important role in molecular self-assembly.

Poster Presentation : **POLY.P-57**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Symmetry breaking of polymer-tethered Au nanoparticles toward helical superstructure in 2D confinement

Seon-Mi Jin, Jun Ho Hwang, Eunji Lee*

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

Organic based nanostructures comprising one-dimensional arrays of gold nanoparticles (Au NPs) are promising materials in sensing, imaging, electronic devices, catalysts, and medical diagnosis due to their unique local surface plasmon resonance (SPR) effect. In particular, helical nanostructures formed by symmetry breaking of NPs closely packed in a confined geometry can improve optical chirality. The NP size, interparticle distance, and uniformity of this distance play an important role in tuning the surface plasmon wavelength and coupling effect. Herein, we explore the helical and zigzag assemblies of polymer tethered Au NPs confined in cylindrical nanochannels of an anodic aluminum oxide (AAO) template. From this result, we emphasize the importance to accurately analyze the sophisticated nanostructures via three-dimensional transmission electron microscopy. In particular, although the assembly structure having different optical properties is determined by the spatial confinement effect according to the molecular weight (Mn) of the polymer, it can be described as different hierarchical structure from the original structure depending on the viewing angle of the assemblies. This study will provide a strategy to control and predict plasmonic properties depending on the Mn of the polymer ligand.

Poster Presentation : **POLY.P-58**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Reversible Shape Transformation of Block Copolymer Particles using Azobenzene-Coated Au Nanoparticles

Seungho Kwon, Meng Xu, Bumjoon Kim*

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

Light-responsive PS-*b*-P2VP/Au NP polymer nanocomposite platforms with controlled nanostructures were developed in a reversible manner. The key idea is to introduce azobenzene-based ligand to the Au NP surface, whose polarity changes reversibly due to the photoisomerization of azobenzene by a specific wavelength of light. Under the visible light, sphere shape BCP particles were generated with well-distributed Au NPs on the PS-outer layer. Otherwise, ellipsoid particles were observed under UV irradiation in which both PS and P2VP blocks were exposed to the surface and Au NPs localized at the PS/P2VP interface. We noted that the azobenzene-coated Au NPs could be modulated the surface wetting behavior of BCP domains by light, inducing the shape transition of colloidal particles and selective localization of Au NPs. We expect the reversible photo-active hybrid systems can be applied in practical applications such as or optical sensor photo-patterning.

Poster Presentation : **POLY.P-59**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Columnar Liquid Crystals for the Helical Assembly and Response to Electric Field: Decisive Role of 1,2,3-Triazolyl Linkers

Manh Linh Nguyen, Byoung-Ki Cho^{1,*}

chemistry, Dankook University, Korea

¹*Department of Chemistry, Dankook University, Korea*

In functional liquid crystal (LC) materials, the design of the functional linker strongly affects not only the morphology but also the physical properties of the material. Recently, owing to its merit of directional hydrogen bonding and large dipole moment (4.55 Debye), 1,2,3-triazole has been utilized as a promising functional linker to the design of helical and electro-responsive liquid crystals. However, in the previous reports of functional liquid crystal based-on 1,2,3-triazolyl, the decisive role of the functional linker may be still questioned. To clarify this argument, we prepared two comparative LC homologs which have a nearly identical molecular structure with the only difference in the identity of the functional linker, i.e. 1,2,3-triazole (1) and 1,3,4-oxadiazole (2). Remarkably, only 1 exhibits the intracolumnar order columnar phase, which is attributed to the head-to-tail hydrogen-bonded network via triazolyl nitrogen and hydrogen atoms. Computer simulation proved that the existence of triazolyl hydrogen atom leads to the tilted conformation of the triazolyl groups with respect to the naphthalene core, which encourages the hydrogen-bonded network, and therefore helical formation. Meanwhile, 2 tend to adopt the co-planar conformation, leading the simple face-to-face stacking, and therefore simple hexagonal column without helical order. Besides, in comparison to 2, the molecular dynamic of 1 is also more flexible as evidenced by the lower rotational energy in simulation and a molecular relaxation mode in dielectric relaxation spectroscopy. Hence, only 1 shows the uniform alignment capability, although both linkers possess a large dipole moment. By this simple material fabrication, the electric conduction of 1 can be improved twice.

Poster Presentation : **POLY.P-60**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Control of the cellular organization by using a robust liquid crystalline nanogroove template

Min Jeong Shin, Dong Ki Yoon*

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

Recently, people in liquid crystals (LCs) field pay their attention to find a correlation between the living cells and LCs after the finding of liquid crystalline order present in biological cells. Even though many commercially available LCs are known to be toxic to the cells, some nature-derived LCs such as cholesteryl ester LCs and cellulose have been recognized as its cell-growing ability. In addition, liquid crystal elastomers(LCEs) have recently exploited as a cell-growing and alignment layer. Hitherto, LC materials reported for the cell growing and alignment template, however, involve a complicated fabrication method or long manufacturing time. Here, we report a semifluorinated liquid crystal material, called Y002, forming nanogrooves as a result of sublimation and recondensation at air-LC boundary. The nanogrooves can be fabricated within less than 30 min. The morphology can be maintained at room temperature and the structure is robust because it is in crystal phase. The nanogrooves can act as a template for growing and aligning NIH-3T3 fibroblast cells after a surface modification with Osmium tetroxide. The surface property of the nanogrooves could be tuned from hydrophobic to hydrophilic, which enables preferential adhesion of the cells. Moreover, the cell organization can be random or uniaxial depending on the alignment of the nanogrooves. Even other cells, including A375 and HeLa cells, could be cultured and aligned on the nanogrooves, proving its universality in other cell lines. The nanogrooves, therefore, show its potential for understanding tissue engineering, cancer tissue migration as well as disease therapies.

Poster Presentation : **POLY.P-61**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Room Temperature Bicontinuous Cubic and Hexagonal Columnar Liquid Crystalline Electrolytes based on non-crystallizable Dendritic Amphiphiles.

Do Thi Huyen, Byoung-Ki Cho^{1,*}

Chemistry, Dankook University, Korea

¹*Department of Chemistry, Dankook University, Korea*

A bicontinuous cubic (Cubbi) liquid crystalline (LC) material mixing with lithium salts is a promising candidate for electrolyte. However, it is generally difficult to obtain the Cubbi phase at room temperature (RT) due to the crystallization, which limits the practical usage of materials. To tackle this issue, we designed a non-crystallizable dendritic amphiphile consisting of branched alkyl chains as an ionophobic part and tri(ethylene oxide) (TEO) coils as an ionophilic part. Herein, two ionic samples showing hexagonal columnar (Colhex) (1) and Cubbi (2) LC phases at RT were prepared by adding different amounts of lithium salt to the amphiphile. The morphology-dependent conduction behavior in ionic samples was investigated by impedance analysis. Notably, the Cubbi phase exhibits a higher ion conductivity in comparison to the Colhex phase. This dominant ionic conduction of the Cubbi phase can be attributed to its 3D ionic networks. In addition to the conduction behavior, Nyquist plot and electric loss can also reveal the phase transition from microphase-separated phase to molecularly mixed liquid phase.

Poster Presentation : **POLY.P-62**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Mechanochemical Synthesis of Reprocessable Biomass-Derived Polyurethane Thermosets and Their Shape-Memory Applications

Inhwan Cha, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

Because of the environmental issues associated with thermoset polymers, recyclable polymers are highly in demand, and the use of sustainable biomass-derived ingredients is also becoming increasingly important. In this work, we utilized 2,5-bis(hydroxymethyl)furan as a starting material to produce network polyurethanes (NPU) under facile, solvent-free (solid-state) ball milling conditions. Urethane bonds may undergo thermally controlled transcarbamoylation, a reversible dynamic covalent bond exchange, enabling reshaping of NPUs. Taking advantage of this chemistry, we demonstrated the self-healing, reprocessing, and shape-memory properties of biomass-derived NPU films using meso-erythritol as a crosslinking agent. Interestingly, in urethane-bond-forming reactions, the relative reactivity of the secondary alcohol group of meso-erythritol over the primary one was remarkably different in the solid state, resulting in NPU films with much enhanced mechanical properties. Dynamic mechanical thermal and stress relaxation analyses indicated that the NPU films possess typical characteristics of vitrimers, such as constant crosslink density and Arrhenius-like reduction in viscosity at elevated temperatures, even though the dissociative exchange of urethane bonds may work here. Our mechanochemical approach is facile and scalable, enabling the preparation of sustainable and recyclable polymers from various biomass-derived chemicals.

Poster Presentation : **POLY.P-63**

Polymer Chemistry

Zoom 2 FRI 15:00~16:00

Synthesis of Furan-based Polyurethanes using a Versatile Polymer Platform via Curtius Rearrangement

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) from biomass sugars, which have good thermal stability, has been considered as a good biomass precursor. Curtius rearrangement is the thermal decomposition of an acyl azide to an isocyanate with a loss of nitrogen gas. Bioplastics are commonly defined as the biobased or biodegradable polymer. To solve environmental pollution, it is important to develop eco-friendly polyurethane with photodegradation ability. In this study, FDCA is substituted with acyl azide and reacts to a variety of alcohols via Curtius rearrangement. Through various catalyst screenings such as DBTDL, DABCO, organic catalyst, optimize the reaction condition. Also, the nitro group was introduced at the ortho position to photo-degradable polyurethane. We measured photo-degradability of synthesized polyurethane and can be applied as eco-friendly plastic.

Poster Presentation : **POLY.P-64**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Self-Healable and Reprocessable Properties of Biomass-Derived Polyurethane Networks "Using" Carbon Dioxide Immobilization

Seohyun Baek, Changsik Song^{1,*}

Polymer Synthesis Lab., Sungkyunkwan University, Korea

¹Department 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. Therefore, 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. We need to focus on environmental issues and to develop and expand the application of green research. Biomass-based vitrimer which have thermal stability and recyclability is suitable for application of eco-friendly polymers. In this study, we synthesized a biomass-derived polyurethane vitrimer (PU vitrimer) using a new furan carbonate diol (FCD-R) in eco-friendly methods. The first method of FCD-R synthesis was direct introduction of carbon dioxide into BHMF, and the second method was to synthesize FCD-R with BICMF. Using mechanochemical synthesis (Ball-milling), the PU vitrimer was made from FCD-R, erythritol, and Hexamethylene diisocyanate (HDI). The film was fabricated using hot press and performed self-healing properties by exchanging dynamic covalent bonds. The thermal properties of the vitrimer were measured by TGA, DSC, DMA, and rheometer. Accordingly, vitrimer, 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-65**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Additive-free photo-mediated oxidative cyclization of pyridinium acylhydrazones to 1,3,4-oxadiazoles: energy level engineering via supramolecular strategy

Kyung-su Kim, Changsik Song*

Department of Chemistry, Sungkyunkwan University, Korea

In this study, we discovered the photo-mediated oxidative cyclization reaction of pyridinium acylhydrazones to 1,3,4-oxadiazole under ambient conditions without a photocatalyst or strong oxidant. This photoreaction proceeded by single electron transfer from excited pyridinium acylhydrazones to oxygen, generating superoxide radical anion (O_2^-). Our findings are remarkable in two ways. First, the additive-free photoreaction proceeded successfully in solid-state microporous organic polymers which contain pyridinium acylhydrazone moieties. Second, the photomediated oxadiazole formation reaction of pyridinium acylhydrazones could be completely inhibited by inclusion complexation with cucurbit[7]uril (CB7) via modulation of electronic states of the acylhydrazones. We believe that such controllable molecular systems will provide diversity and applicability for the development of smart materials.

Poster Presentation : **POLY.P-66**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Humidity-Responsive Liquid Crystal Elastomers Prepared by Surface Alignment and Direct Ink Writing

Keumbee Kim, Suk-kyun Ahn^{1,*}

Department of Chemical Engineering, Pusan National University, Korea

¹*Department of Polymer Science and Engineering, Pusan National University, Korea*

Herein, we present a new class of humidity-responsive liquid crystal elastomer (LCE) incorporating dimethylamino moieties that can be prepared by versatile processing, including surface alignment as well as 3D printing. The humidity-responsive properties are introduced by activating one of the LCE surfaces with an acidic solution, which generates cations on the surface, and provides asymmetric hydrophilicity to the LCE. The resulting humidity-responsive LCE undergoes programmed and reversible hygroscopic actuation, and its shape transformation can be directed by the cut angle with respect to a nematic director or by localizing activation regions in the LCE. Most importantly, various humidity-responsive LCE actuators, including a flower, a concentric square array, and a soft gripper, are successfully fabricated by employing LC inks in direct-ink-writing 3D printing.

Poster Presentation : **POLY.P-67**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Norbornene-based bottle-brush polymers: synthesis and hydrated lubricating properties

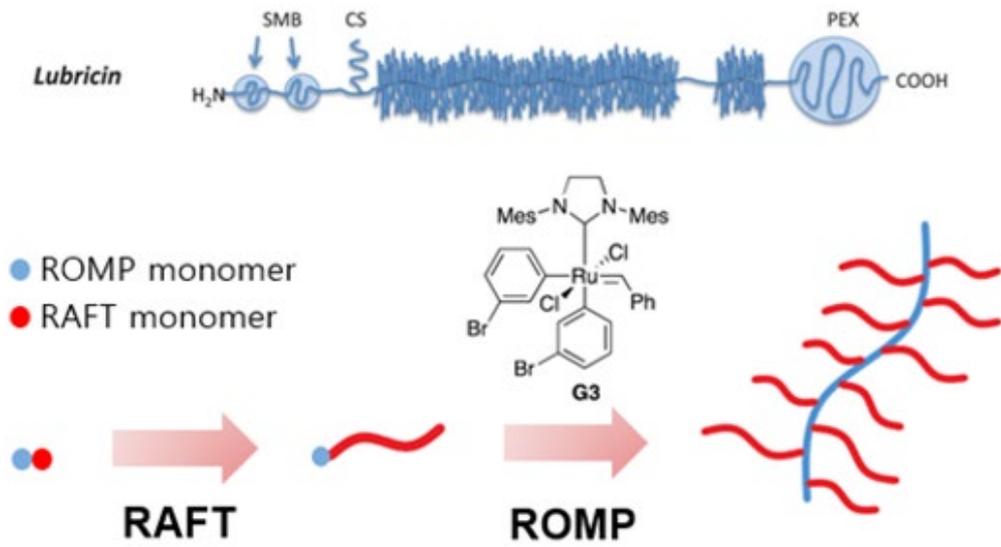
Hwi Hyun Moon, Changsik Song^{1,*}

Sungkyunkwan University, Korea

¹*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 (cationic, anionic, or zwitterionic) were used for ROMP and RAFT, respectively. The reactions were carried out by tuning Grubb's catalyst generation, the concentration of Grubb's catalyst, the amount of initiator, and solvents. 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.

Biomimetic bottle-brush polymer inspired by lubricin



Poster Presentation : **POLY.P-68**

Polymer Chemistry

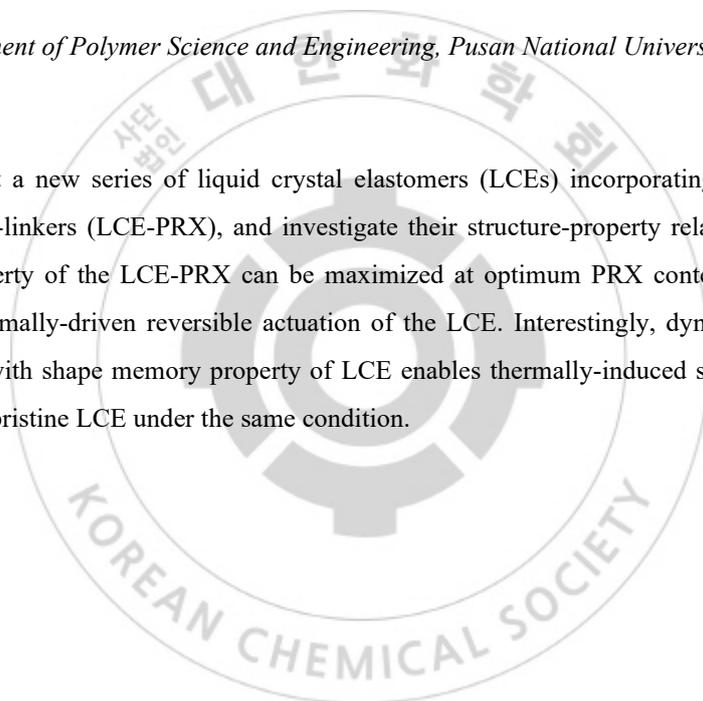
Zoom 2 FRI 16:00~17:00

Liquid Crystal Elastomers Incorporating Slide-Ring Polyrotaxane Cross-linkers: Mechanical Properties, Actuation and Self-Healing

Subi Choi, Suk-kyun Ahn*

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

Herein, we present a new series of liquid crystal elastomers (LCEs) incorporating various amount of polyrotaxane cross-linkers (LCE-PRX), and investigate their structure-property relationship. Toughness and damping property of the LCE-PRX can be maximized at optimum PRX content (0.5 wt%), while preserving the thermally-driven reversible actuation of the LCE. Interestingly, dynamic nature of PRX crosslinker along with shape memory property of LCE enables thermally-induced self-healing, which is ineffective for the pristine LCE under the same condition.



Poster Presentation : **POLY.P-69**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Covalent Adaptable Liquid Crystal Elastomers with Poly(ether-thiourea) Crosslinker

Jin-Hyeong Lee, Suk-kyun Ahn*

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

The incorporation of dynamic covalent bonds within liquid crystal elastomers (LCEs) can bring great benefits including reprocessability, shape reprogrammability and self-healing which are not allowed in the conventional LCEs. In this study, we present a new class of reprocessable and reprogrammable LCEs using poly(ether-thiourea) crosslinkers. Interestingly, the thiourea linkages undergo a dissociation above 120 oC evidenced by FT-IR investigation. By exploiting the dynamic nature of poly(ether-thiourea) crosslinker, we successfully demonstrate that the reprocessability of the LCE by compression molding, and the reprogrammability of the permanent shape by mechanical manipulation at elevated temperature, while preserving the capability of reversible actuation.

Poster Presentation : **POLY.P-70**

Polymer Chemistry

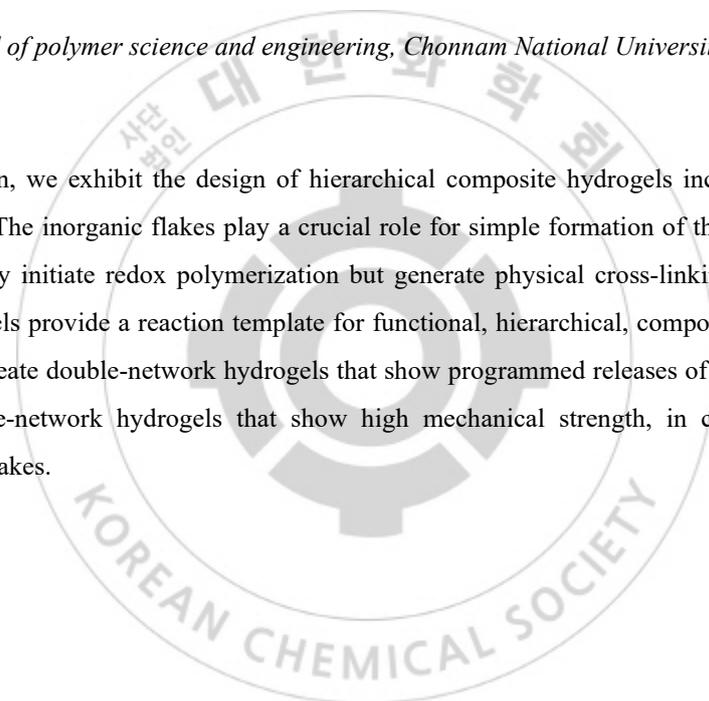
Zoom 2 FRI 16:00~17:00

Synthesis of MoS₂-Embedded Hierarchical Composite Hydrogels that Show Controlled Release and Tunable Mechanical Strength

Songah Jeong, Hyungwoo Kim*

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

In this presentation, we exhibit the design of hierarchical composite hydrogels including molybdenum disulfide (MoS₂). The inorganic flakes play a crucial role for simple formation of the hydrogel networks since they not only initiate redox polymerization but generate physical cross-linking, and the resultant composite hydrogels provide a reaction template for functional, hierarchical, composite hydrogels. Thus, we were able to create double-network hydrogels that show programmed releases of cargo molecules and further form triple-network hydrogels that show high mechanical strength, in conjunction with the embedded MoS₂ flakes.



Poster Presentation : **POLY.P-71**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Multi-color tunable electrofluorochromic materials using pH sensitive ESIPT molecules in PVA hydrogel

Kyeong-Im Hong, Hyun Seo Ahn, Woo-Dong Jang*

Department of Chemistry, Yonsei University, Korea

Electrofluorochromic (EFC) materials are attractive to develop smart materials such as smart windows, sensing devices, actuators, and anticounterfeiting devices. Most of them were consisting with fluorophores and redox-active derivatives such as triphenylamine and triphenylborane. Their absorption/emission colors were usually turned on or off by the application of an electric field. Recently, pH sensitive fluorescent materials were employed for electrofluorochromic devices through proton coupled electron transfer. It could be more useful to construct the multi-functional EFC devices with various emission colors. We have recently demonstrated several ESIPT molecules successfully showed EFC properties by means of pH sensitive properties. We expanded these properties to develop EFC materials with wide range of emission colors. ESIPT molecules showed large Stokes shift and AIE in solid state. The synthesized ESIPT molecules were embedded on PVA hydrogel to construct the practical materials. Their emissions were maintained in PVA hydrogel and also tuned by the application of an electric field. As a result, we have finally suggested that PVA hydrogel containing ESIPT molecules would be efficiently applied to smart materials. Detailed aspect of this system will be presented in this symposium.

Poster Presentation : POLY.P-72

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

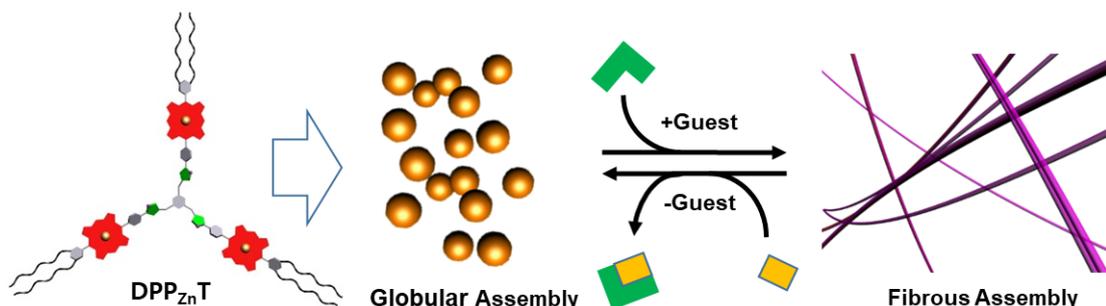
Guest-triggered supramolecular polymerization and depolymerization of triazole-bearing porphyrin tripod

Hosoowi Lee, Woo-Dong Jang^{1,*}

Department of Chemistry, College of Science, Korea

¹*Department of Chemistry, Yonsei University, Korea*

A triazole-bearing tripodal porphyrin (**DPP_{Zn}T**) was designed as a monomeric building block for supramolecular polymer, which formed spherical nanoparticles. When **DPP_{Zn}T** solution in toluene was spin-coated onto mica surface, the formation of spherical nanoparticles was observed by atomic force microscopy (AFM). UV/Vis spectral titration using structural fragments of **DPP_{Zn}T** and molecular modelling study reveals that the axial coordination of triazole groups to zinc(II) porphyrin wings are suppressed due to the steric hindrance. UV/Vis spectral titration of **Py₃B** to **DPP_{Zn}T** indicated the formation of 1:1 host-guest complex between **Py₃B** and **DPP_{Zn}T** (**DPP_{Zn}T**·**Py₃B**) having cone-shape geometry. AFM and transmission electron microscopy (TEM) observation of **DPP_{Zn}T**·**Py₃B** clearly showed the formation of fibrous supramolecular polymers. The addition of Cl⁻ to **DPP_{Zn}T** also triggered the transformation from spherical nanoparticles to fibrous supramolecular polymer. Furthermore, once formed fibrous supramolecular polymer was recovered to original spherical nanoparticle by the treatment of Cu(ClO₄)₂ and AgNO₃ to remove **Py₃B** and Cl⁻, respectively.



Poster Presentation : **POLY.P-73**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Preparation of water-based eco-friendly powder type polyimide composite separator

Hyun Soo An, Chan-Moon Chung^{1,*}

Department of Chemistry, Yonsei university, Korea

¹*Department of Chemistry, Yonsei University, Korea*

In recent years, lithium ion batteries have been developed with high performance for electric devices of vehicles. As one important part of lithium ion battery, separator is used to prevent explosion by blocking the contact between the anode and the cathode, and serves as a channel for ions. Because the traditional polyethylene separator has poor thermal properties, various studies have been conducted to meet the requirements for more stable separator properties by surface treatment or coating. Polyimide separators for lithium ion batteries mostly are studied as nano-fiber membranes by treating poly(amic acid) under high voltage electrospinning and high temperature imidization conditions. In the conventional study on polyimide separator, organic solvents are used, and they are not environmentally friendly. In addition, in the case of using electrospinning, it is difficult to expect economical or time efficiency. In this study, polyimide synthesized in water is obtained in the form of a powder. Coating slurry is prepared with a water-soluble binder. It aims to improve thermal and mechanical properties by coating on polyethylene separator. All of these processes aim to be thoroughly conducted in the water system that do not use harmful organic solvent. Also, Using a relatively efficient and simple coating process and effective control of coating thickness are also an advantage.

Poster Presentation : **POLY.P-74**

Polymer Chemistry

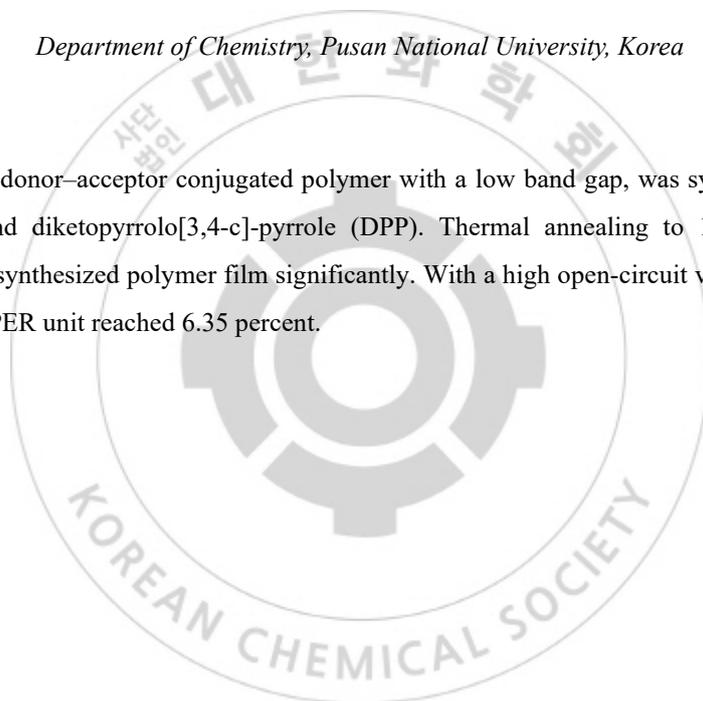
Zoom 2 FRI 16:00~17:00

Perylene and diketopyrrolopyrrole are used to create a highly crystalline low-band-gap polymer for organic photovoltaic cells

Seon Lee Gwak, Do-Hoon Hwang*

Department of Chemistry, Pusan National University, Korea

PDPP-PER, a new donor–acceptor conjugated polymer with a low band gap, was synthesized using 3,9-perylene (PER) and diketopyrrolo[3,4-c]-pyrrole (DPP). Thermal annealing to 150°C increased the crystallinity of the synthesized polymer film significantly. With a high open-circuit voltage of 0.79 V, the PCE of the PDPP-PER unit reached 6.35 percent.



Poster Presentation : POLY.P-75

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

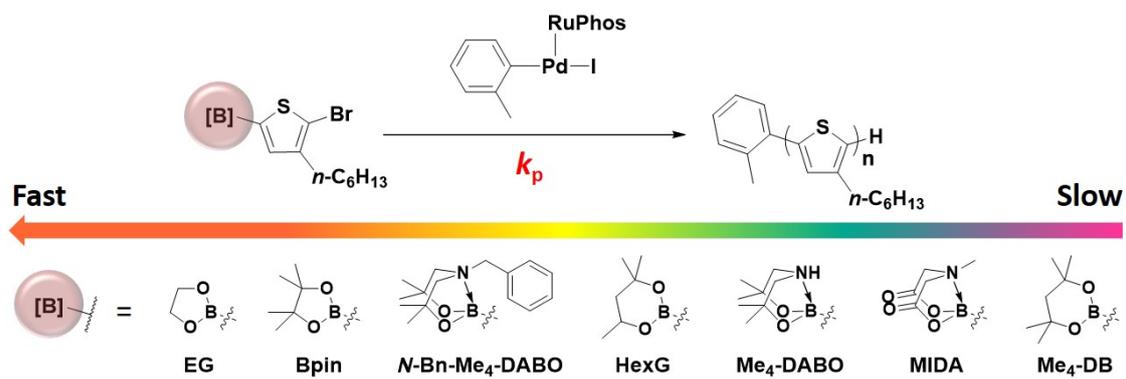
Tuning Boron Reagent Enables Modulation of the Rate of Polymerization in the Precision Synthesis of Poly(3-Hexylthiophene): Realization of One-Shot Gradient Copolymerization

Hyunwoo Park, Tae-Lim Choi^{1,*}

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

Despite the great breakthrough in the Catalyst-transfer polycondensation (CTP) using various organometallic monomers (Grignard, organotin, organozinc) for the controlled synthesis of conjugated polymers, modulating the reactivity was limited from the narrow scope of the organometallic functional groups. We herein report the expanded scope of boron functional groups in the Suzuki-Miyaura cross-coupling mediated CTP (SCTP) of 3-alkylthiophenes and investigate the relationships between their structure, reactivity and control. First, cyclic boronic esters of 6-membered ring (compared to 5-membered ring analogues) and with larger number of α -methyl substituents showed lower k_p (rate constant of propagation). Next, by modifying the *N*-methyliminodiacetic acid (MIDA) boronate structure, we found that *N*-coordinated boronate with α -methylene substituents in place of the carbonyl substituents showed higher k_p , and those with α -gem dimethyl substituents and smaller *N*-substituent showed lower k_p in correlation to the N→B bond length. As a result, the reactivity of 3-alkylthiophene based monomer could be tuned. For each set of cyclic boronic esters or *N*-coordinated boronates, boron reagent of lower k_p underwent lower degree of side reactions such as chain transfer or homocoupling and yielded the polymers of higher end-group fidelity with narrower dispersity. Poly(3-hexylthiophene) (up to 11.7 kg/mol) were synthesized with excellent control and yield (>90%). Finally, utilizing two different boron reagents, we demonstrate the successful synthesis of gradient copolymer poly(3-hexylthiophene)-*grad*-poly(3-(2'-ethylhexyl)thiophene) by one-shot copolymerization.



Poster Presentation : **POLY.P-76**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

A 3D interconnected network of MCNT/polyacrylic hydrogel and its EMI shielding behavior at different pH condition

Daewon Sohn^{*}, Quyen Vu Thi

Department of Chemistry, Hanyang University, Korea

Considering the rapid development of wireless technology with various electronic devices, multi-band satellite communication, and ultra-wideband radars, it is urgent to design an efficient material that exhibits high absorbance with a large frequency range to eliminate the significant increase of electromagnetic pollution. In this work, a 3D network of multi-walled carbon nanotubes (MCNT) and polyacrylic acid (PAA) hydrogel was prepared by free radical polymerization method by varying filler content of MCNT at 1, 2, and 3 wt%. The PAA polymeric chains were successfully formed along the MCNT tube, resulting in an increase in the diameter of MCNT. The composite hydrogel showed a remarkable enhancement in a chemical property where the breaking stress was 7.4 times higher than its value in pristine PAA hydrogel at only 3wt% content of MCNT. The MCNT/PAA hydrogel exhibited excellent EMI shielding performance in X range frequency from 8.2 to 12.4 GHz. Interestingly, the total shielding efficiency (SET) is higher at lower pH conditions owing to the higher ionic conductivity. The SET was about 32.8 dB at pH 3.5 and reached up to 41.1 dB at pH of 0.5 at the shielding thickness of only 2.5 mm. This work is expected to provide a promising method for developing high-performance shielding material starting from the 3D network of MCNT/hydrogel composite.

Poster Presentation : **POLY.P-77**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Efficient Green-Emitting Perovskite Light Emitting Diodes based on Perovskite-Conjugated Polyelectrolytes Emitters

Amit Kumar Harit, Han Young Woo^{1,*}

Department of Chemistry, Korea University, India

¹*Department of Chemistry, Korea University, Korea*

Charge carrier confinement and defect passivation are main concerns in the development of solution-processed perovskite light-emitting diodes (PeLEDs). Here, we present a green-emitting PeLED by compositing an anionic conjugated polyelectrolyte (MPS2-TEA) and quasi-2D perovskite based on formamidinium lead tribromide. Atomic force microscopy and scanning electron microscopy images show perovskite films with MPS2-TEA show a reduced root-mean-square roughness and reduced grain sizes compared to the films without MPS2-TEA. Increased photoluminescence intensity (by 3 times) and lifetime (18.11 vs 9.81 ns) of perovskite films with MPS2-TEA compared to pristine films suggest the improved radiative recombination by intermixing perovskite and MPS2-TEA. Space-charge-limited current measurements reveal the significantly suppressed defect density ($3.94 \times 10^{17} \text{ cm}^{-3}$) in perovskite films with MPS2-TEA due to defect passivation at grain boundaries by MPS2-TEA. The composite PeLED shows a significantly improved external quantum efficiency up to 15.47% (9.28% without MPS2-TEA) together with a maximum luminance (12,252 cd m^{-2}) and current efficiency (69.02 cd A^{-1}).

Poster Presentation : **POLY.P-78**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Effect of Crosslinking on the Mechanical and Thermal Properties of Polyimide/Hexagonal Boron Nitride Nanocomposite Film

Dam bi Kim, Chan-Moon Chung*

Department of Chemistry, Yonsei University, Korea

Polyimide (PI) is an engineering plastic that is widely used in various devices owing to its good mechanical properties, flexibility, excellent thermal stability, low dielectric permittivity and chemical resistance. Recently, owing to the demands in denser and faster circuits in electronic devices, the dissipation of heat generated in electronic components has attracted more attention and is considered as a critical issue to be resolved. To solve the heat dissipation problem, various fillers were used as the thermal conductive materials embedded in a polymer matrix. Among them, hexagonal boron nitride (h-BN) has the greatest potential due to its high thermal conductivity (up to 400 W/m·K) and relatively low dielectric constant. In this study, a boron nitride-based crosslinked polyimide (PI-BN) nanocomposite was prepared as heat dissipation materials (composed of a h-BN and a PI derived from 4,4'-(hexafluoroisopropylidene)diphthalic anhydride (6FDA), 2,2-bis[4-(4-aminophenoxy)phenyl]propane (BAPP) and 3,5-diaminobenzoic acid (DABA)). Chemical crosslinking of PI may provide feasible routes for the improvement of the mechanical properties and thermal stability. The thermal conductivity and tensile strength according to the crosslinking density of PI and the content of BN were evaluated.

Poster Presentation : POLY.P-79

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Electrochemical and morphological characteristics of chalcogenophenes (furan, thiophene, and selenophene) on Cyclopentadithiophene and benzo-thiadiazole based backbone.

Mingi Sung, Junghoon Lee^{1,*}

Energy and Biotechnology, Dongseo University, Korea

¹*Dongseo University, Korea*

As we have known, the extended π -conjugated structure facilitates charge transport in the device by facilitating orbital bonds between molecules that determine the size of the charge transfer integral. Moreover, better intermolecular charge hopping and intramolecular charge transport depend on better morphology of the conjugated materials. Three chalcogenophenes (furan, selenophene and thiophene) combine with Cyclopentadithiophene(CDT) as a donor and fluoro-benzothiadiazole(FBT) as an acceptor based backbone. CDT-FBT based donor (D)-acceptor (A) monomers with various heteroacene-type (thiophene (Th), selenophene (Se), and furan (O)) donor rings has been designed and synthesized as a means to systematically understand structure-property relationships on the subject of the effect of chalcogen elements in donor portions for applications in OFETs. The electronic properties of these materials were examined by cyclic voltammetry and UV-vis spectroscopy. To determine the molecular arrangement of this polymer, GIWAXS (Grazing incidence wide angle x-ray scattering) was measured. CFC-O, CFC-S, and CFC-Se all showed an increase in the degree of polymer alignment when comparing before and after heat treatment using atomic force microscope(AFM). The effective mobility of electrons and holes is 0.06, 0.14 and 0.19 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$, respectively.

Poster Presentation : **POLY.P-80**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Alkyl Chain Engineering on a New “Y-series” Non-Fullerene Acceptor for Organic Solar Cells

Kyungmin Sung, Sung-Ho Jin^{1,*}

Department of Chemical Materials, Pusan National University, Korea

¹Department of Chemical Education, Pusan National University, Korea

Since recent emergence of “Y-series” non-fullerene acceptors (NFAs), the field of organic solar cells (OSCs) began to show high power conversion efficiencies (PCEs). Here in, we synthesized two NFAs based on the n-hexyl side chain on triazole moiety. Two NFAs are with (BTA-UD-4F) and without (BTA-4F) alkyl chain on thiophene rings. The decomposition temperature (T_d , at 5% weight loss) were exhibited 280 and 292 °C for BTA-UD-4F and BTA-4F, respectively. The highest occupied molecular orbital of BTA-4F and BTA-UD-4F was exhibited -5.53 and -5.40 eV, respectively. The lowest unoccupied molecular orbital of BTA-4F and BTA-UD-4F was exhibited -4.05 and -3.91 eV, respectively. Therefore, BTA-4F blended with polymer PM7 exhibited a PCE of 8.26 %, open-circuit voltage (V_{oc}) of 0.76 V, a short-circuit current density (J_{sc}) of 18.04 mA/cm², and fill factor (FF) of 62.23%. BTA-UD-4F blended with polymer PM7 exhibited a PCE of 9.12 %, V_{oc} of 0.71 V, J_{sc} of 21.08 mA/cm², and FF of 62.04%. BTA-UD-4F showed better device performance compared to BTA-4F.

Poster Presentation : **POLY.P-81**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Benzotriazole Based Siloxane Side Chains Polymer for Non-fullerene Organic Solar Cells

Hyungjin Park, Sung-Ho Jin^{1,*}

Department of Chemical Materials, Pusan National University, Korea

¹*Department of Chemical Education, Pusan National University, Korea*

The new polymer Nap-SiBTz is designed and synthesized for fabrication of non-fullerene organic solar cells (NFOSCs) application. Nap-SiBTz comprised of 4,8-bis(5-(6-((2-hexyldecyl)oxy)naphthalen-2-yl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene (BDT) as donor and 4,7-bis(5-bromo-6-undecylthieno[3,2-b]thiophen-2-yl)-5,6-difluoro-2-(6-(1,1,1,3,5,5,5-heptamethyltrisiloxan-3-yl)hexyl)-2H-benzo[d][1,2,3]triazole (SiBTz) as acceptor. The Nap-SiBTz was synthesized by Stille polymerization. The thermal, photophysical and electrochemical properties of Nap-SiBTz were systematically investigated. Interestingly, Nap-SiBTz exhibited wide band gap (E_g) of 1.91 eV with highest occupied molecular orbital (HOMO) = -5.25 eV and lowest unoccupied molecular orbital (LUMO) = -3.34 eV, and showed better compatibility with ITIC as non-fullerene acceptor. The Nap-SiBTz was thermally stable up to 408 °C as revealed by its thermogravimetric analysis (TGA) (5% weight loss). Therefore, Nap-SiBTz blended with ITIC exhibited a efficiency of 4.76 %, open-circuit voltage (V_{oc}) of 0.77 V, a short-circuit current density (J_{sc}) of 11.60 mA/cm², and fill factor (FF) of 53.18%, respectively. This results indicated that benzotriazole based siloxane side chain polymer have great potential to further development of NFOSCs.

Poster Presentation : **POLY.P-82**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

Anthracene Based Novel Fluorescent Materials for Deep-Blue Organic Light-Emitting Diodes with High-Color-Purity

Kumaresan Raja, Sung-Ho Jin^{1,*}

Department of Chemical Materials, Pusan National University, India

¹*Department of Chemical Education, Pusan National University, Korea*

Anthracene based emitters were designed and synthesized for deep-blue fluorescent organic light-emitting diodes (OLEDs), namely, CZm-AN-mPO, CZ-AN-PO, PyIN and PyOUT, respectively. Their photophysical, thermal, electrochemical and electroluminescence (EL) properties are systematically investigated. All four deep-blue emitters exhibited intense deep-blue emission with a narrowed full width half maximum (FWHM) in solution and thin film-state at room temperature. The emitters showed excellent thermal stability over 400 °C. Principally, the device using CZ-AN-PO as emissive layer exhibited a maximum external quantum efficiency (EQEmax) of 7.3 % and FWHM of 52 nm with deep-blue Commission Internationale de L'Eclairage coordinates (CIEx,y) of (0.15, 0.07). Additionally, we achieved EQEmax of 4.3 and 4.0 % with CIEx,y of (0.15, 0.15) and (0.16, 0.17) for PyIN and PyOUT, respectively. These results reveals that anthracene derivatives are very close to the National Television System Committee (NTSC) recommended CIE deep-blue color coordinate (0.14, 0.08).

Poster Presentation : **POLY.P-83**

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

A New Benzodithiophene π -Conjugated Polymer with Hexylbenzene Side Chain for Organic Photovoltaics

Durgagayathri Rajarapati, Sung-Ho Jin^{1,*}

Department of Chemical Materials, Pusan National University, India

¹Department of Chemical Education, Pusan National University, Korea

The new benzodithiophene (BDT) based π -conjugated donor-acceptor polymer (PBDT-Cl) is synthesized with the side chain modification and explored as donor for organic photovoltaics (OPV). The thermal, electrochemical and optical properties of PBDT-Cl were studied systematically. The hexyl benzene side chain introduction on BDT core showed good absorption profile ranging from 300-750 nm with $E_{\text{gopt}} = 1.85$ eV, and exhibited better solubility in halogenated and non-halogenated solvents. The organic solar cell(OSC)s were fabricated with PBDT-Cl as donor and IT-4F as acceptor showed power conversion (PCE) of 4.02%. PBDT-Cl showed comparatively high fill factor and short circuit current density when fabricated along with Y6 compared to IT-4F as acceptor. These results suggest that the new polymer has a great ability for enhancing efficiency, which will provide new routes for the development of new class of polymers for high-performance air-stable OSCs.

Poster Presentation : POLY.P-84

Polymer Chemistry

Zoom 2 FRI 16:00~17:00

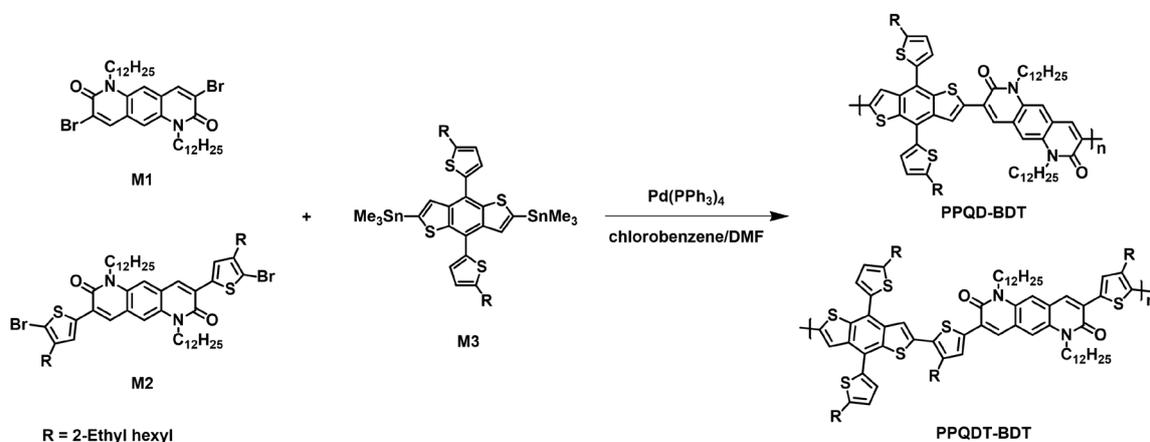
Synthesis and Characterization of Lactam-based Novel Acceptor Unit for Organic Solar Cells(OSCs)

Suha Lee, Do-Hoon Hwang^{1,*}

Department of chemistry, Pusan National University, Korea

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

We synthesized new lactam-based acceptor unit, pyrido[2,3-g]quinoline-2,7(1*H*, 6*H*)-dione (PQD) and using this acceptor unit, two lactam-based polymers, poly(3-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-*b*:4,5-*b'*]dithiophen-2-yl)-1,6-didodecylpyrido[2,3-*g*]quinoline-2,7(1*H*,6*H*)-dione) (PPQD-BDT) and poly(3-(5-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-*b*:4,5-*b'*]dithiophen-2-yl)-4-(2-ethylhexyl)thiophen-2-yl)-1,6-didodecyl-8-(4-(2-ethylhexyl)thiophen-2-yl)pyrido[2,3-*g*]quinoline-2,7(1*H*,6*H*)-dione) (PPQDT-BDT), with or without thiophene spacer were finally synthesized and characterized their optical, electrochemical properties. Two polymers have wide-band gap energy level about 1.90 eV with a maximum absorption at 550 nm. To understand photovoltaic performance of two polymers, we fabricated photovoltaic devices with inverted structure. As a result, PPQDT-BDT showed better performance, a PCE of 2.86% with a J_{SC} of 7.54 mA/cm²



Poster Presentation : **IND.P-85**

Industrial Chemistry

Zoom 19 FRI 16:00~17:00

Solidification/stabilization of Carbonates via Metakaolin-Based Geopolymer

Hyung-Ju Kim

Decommissioning Technology Research Division, Korea Atomic Energy Research Institute, Korea

Carbowastes originated from decommissioning of nuclear power plant include the ^{14}C as major nuclides. To significantly reduce the amount of carbowastes, thermochemical treatment is frequently applied, thereby radioactive CO_2 coming out while the activity of remaining wastes goes below clearance level. Then, the newly produced radioactive CO_2 can be captured by mineral carbonation technology which generates carbonates as final product. Next, the solidification/stabilization (S/S) process is inevitably required to safely store the concentrated ^{14}C at disposal site. Diverse solidification agents are utilized for S/S process depending on the type of wastes. Since the decomposition temperature of carbonates is around $600\text{ }^\circ\text{C}$, the room temperature S/S process is preferred to avoid potential danger. Thus, metakaolin-based geopolymerization is selected which can overwhelm the solidification quality of conventional cementation. In this presentation, we present the successfully fabricated the solidification via metakaolin-based geopolymer with carbonates loading up to 60 wt%. The solidification quality is evaluated with respect to the acceptance criteria of disposal site. The effect on different carbonates, alkaline activator is also elucidated with physicochemical characterizations of solidifications.

Poster Presentation : **IND.P-86**

Industrial Chemistry

Zoom 19 FRI 16:00~17:00

IrS : Photophysical Properties of Homoleptic Ir(III) Complexes with N-dibenzothiophenyl-N-imidazole Ligands and its Application in OLEDs

Sanghun Lee, Daehan Lee, Min Su Choe, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

The NHC-Ir complexes **f-IrS^{iPr}**, **m-IrS^{iPr}**, and **m-IrS^{Me}**, in which a dibenzothiophene (DBT) moiety is used to increase the emission efficiency for deep blue phosphorescence, were synthesized and compared with the dibenzofuran (DBF)-based Ir complexes **f-IrO^{Me}** and **m-IrO^{Me}**. The differences in the ligand structure (DBF/DBT) or configuration (fac/mer) of these complexes led to different electrochemical and photophysical properties. The DBF moiety has different aromaticity than DBT because the electronegativity of the sulfur atom is weaker than that of the oxygen atom and DBT is involved in extended intramolecular conjugation, resulting in a larger T₁-S₀ energy gap and shorter emission wavelength than that of the DBT complexes. On the other hand, the meridional isomer has a mutually trans-phenyl ligand configuration that leads to a lengthening of the transoid Ir-C bond and destabilizes the HOMO level, resulting in greater ease of oxidation, and the emission is red-shifted relative to the facial forms. Even with the differences in the origin of phosphorescence, replacement of the oxygen atom in the DBF unit with sulfur does not greatly alter the emission efficiency in either solution or film, while achieving the same high-end deep-blue phosphorescence with unprecedented CIE coordinates of [0.14,0.19] for **m-IrS^{Me}** (EQE_{max}; 17.1%) and [0.14,0.14] for **m-IrO^{Me}** (EQE_{max}; 18.2%).

Poster Presentation : **IND.P-87**

Industrial Chemistry

Zoom 19 FRI 16:00~17:00

Triazole : Comprehensive Photophysical Elucidation of NHC-Ir Complexes with Triazolophenanthridine Derivatives for Highly Efficient Blue PhOLED

Sanghun Lee, Min Su Choe, Yunjeong Seo, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Triazolophenanthridine-based isomeric NHC-Ir complexes, **Ir(Phenyl)**, **Ir(Tolyl)**, and **Ir(Xylenyl)** were isolated, and systematic investigation of their photophysical properties was carried out. The crystal structures of each Ir complex were determined, and it was found that the meridional isomer of **Ir(Phenyl)** was not formed but **hetero-Ir(Phenyl)** was formed by structural characteristics. Cyclic voltammograms (CV) and density-functional theory (DFT) calculations supported that **hetero-Ir(Phenyl)** has a different electronic structure compared to homoleptic Ir complexes. In the case of homoleptic complexes, orbitals are located in the metal and phenyl part of phenanthridine in HOMO, and in the entire phenanthridine in LUMO. On the other hand, **hetero-Ir(Phenyl)** has orbital distribution extended to the phenyl moiety, where the HOMO is located in the metal and phenyl moiety, and LUMO is located in the phenanthridine. As a result, the energy of **hetero-Ir(Phenyl)** was stabilized and red-shifted emission due to the difference in ligand binding. Finally, all Ir complexes were applied to blue PhOLED as dopant materials and the fabricated device exhibited efficient blue emission. In particular, **hetero-Ir(Phenyl)** showed relatively higher efficiency with an external quantum efficiency (EQE) of up to 16.2%. Similar to the properties in the solvent, the facial isomer was closer to the deep-blue emission because the second peak of the EL spectra was lower than the meridional isomer.

Poster Presentation : **IND.P-88**

Industrial Chemistry

Zoom 19 FRI 16:00~17:00

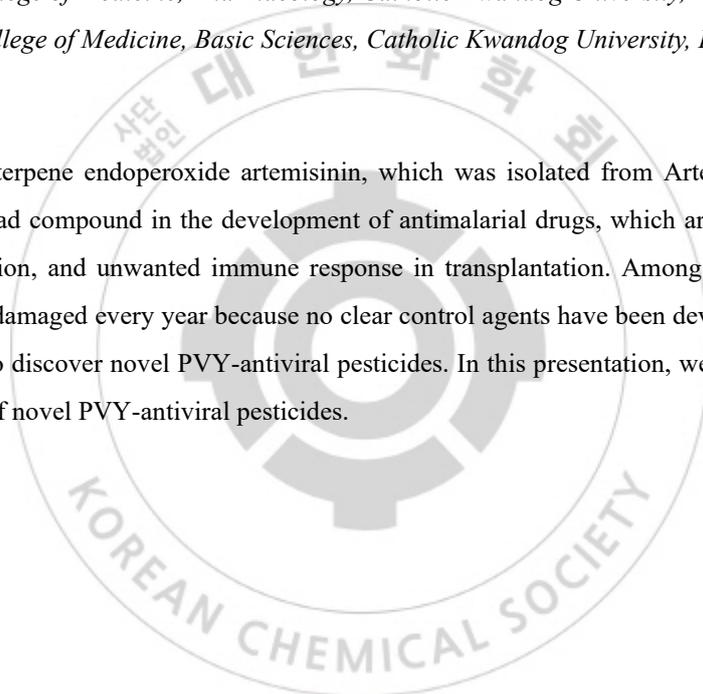
Synthesis of novel PVY-antiviral pesticides from natural artemisinin

Seok Joon Lee^{*}, Sangtae Oh¹

College of Medicine, Pharmacology, Catholic Kwandong University, Korea

¹*College of Medicine, Basic Sciences, Catholic Kwandong University, Korea*

The natural sesquiterpene endoperoxide artemisinin, which was isolated from *Artemisia annua* L., has become a useful lead compound in the development of antimalarial drugs, which are a variety of tumor, viral, fungal infection, and unwanted immune response in transplantation. Among plant diseases, viral diseases are being damaged every year because no clear control agents have been developed. Therefore, it is very important to discover novel PVY-antiviral pesticides. In this presentation, we will show synthesis and antiviral effect of novel PVY-antiviral pesticides.



Poster Presentation : **INOR.P-89**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Self-Assembling Behavior of Porphyrin-Based Supramolecular Polymers in Water

Sukyoung Kim, Sung Ho Jung^{1,*}, Jong Hwa Jung*

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¹Liberal Arts/Chemistry, Gyeongnam National University of Science and Technology, Korea

Self-assembling processes inspired by a biomolecular system is powerful chemistry protocol to organize molecular building-blocks into functional materials with complexity. Recently, the synthetic approaches emerged from a kinetic point of view allows us to investigate the dynamic supramolecular polymerization. Herein, we report the synthesis of Zn- and Cu-porphyrin-based supramolecular polymers. The self-assembling behavior of supramolecular polymers was investigated through temperature-dependent absorption changes in water. Interestingly, the H- and J-aggregates were observed depending on central metal in water. In addition, the 2D nanosheets of Zn- and Cu-porphyrins were formed, its aggregation modes contributed to different heights. We will discuss the influence of axial coordination bonding to Zn- and Cu-porphyrins on supramolecular polymerization.

Poster Presentation : **INOR.P-90**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Regulation of optimal activities of sMMO through the modification of O₂ and C-H activation

Yunha Hwang, Seung Jae Lee^{*}, Dong-Heon Lee

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

The specific enzymatic activities of sMMO are widely investigated to understand its enzymatic activity and turnover rate to understand the influence by substrates including hydrocarbons, molecular oxygen, electrons, and proton. The ratio between substrates and enzymes need to be further investigated to understand its possible influences during expression of hydroxylase and other auxiliary enzymes. In this presentation, the expression of MMOH is described based on the ratio of two substrates including methane and molecular oxygen. The expression level in sMMO is important for the purification of this homodimer ($\alpha_2\beta_2\gamma_2$) and the complex formation of six subunits needs to discover further mechanism studies through MMOG. The methane oxidation is performed in α -subunit of MMOH and β -subunit generates specific interactions for the dimeric formation of hydroxylase component. The function of γ -subunit is not well quite understood, but this small-subunit only detected in water-soluble region after cell-lysis. The methane concentration of sMMO proved that the injection volume of methane and molecular oxygen (O₂) affect the volume of soluble portion of MMOH based on the quantitative analysis. In addition, the differences of these species depend on the concentration of γ -subunit. The specific enzyme activities are also affected by the concentration of methane and oxygen in buffer. The catalytic activities of enzymes are influenced by the ratio of reductase components and high concentration of oxygen decrease the activities.

Poster Presentation : **INOR.P-91**

Inorganic Chemistry

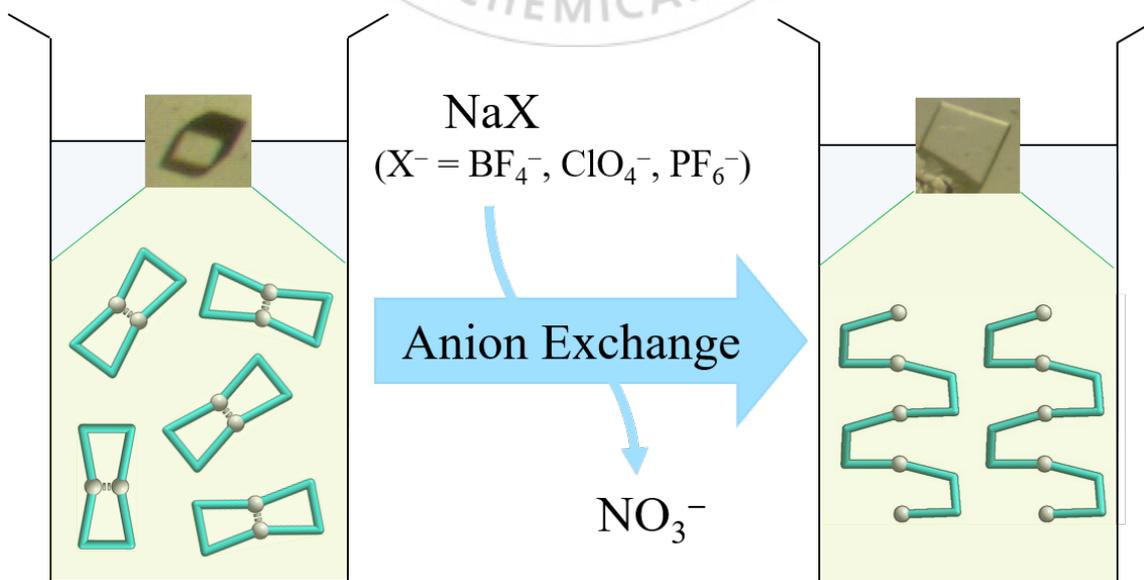
Zoom 3 FRI 15:00~16:00

Supramolecular Isomerism between Cyclodimeric and 1D Coordination Polymers: Competition of Argentophilic vs. Electrostatic Interaction

Heehun Moon, Geon Woo Gwak, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Systematic supramolecular isomerism between metallacyclodimeric species and sinusoidal 1D coordination polymers was observed. Slow diffusion of AgX ($X^- = \text{NO}_3^-$, BF_4^- , ClO_4^- , and PF_6^-) with 1,3-bis(dimethyl(pyridin-4-yl)silyl)propane afforded 28-membered metallacyclodimers $[\text{Ag}(\text{L})_2(\text{X})_2]$ with argentophilic, electrostatic, and π - π interaction that are very sensitive to the bite size of each anion in the crystalline state. Successive anion exchange of $[\text{Ag}(\text{L})_2(\text{NO}_3)_2]$ with X^- ($X^- = \text{BF}_4^-$, ClO_4^- , and PF_6^-) crystallized *in situ*, resulting in a systematic supramolecular isomerization to sinusoidal 1D coordination polymers in mother liquor. In the following pages, the different photophysical properties between the metallacyclodimeric species and the sinusoidal 1D coordination polymers on some solvent adsorption are discussed based on the photoluminescence (PL) spectra.



Poster Presentation : **INOR.P-92**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Engineering of reductase domains through FAD binding and ferredoxin domains

Chae Min Lee, Seung Jae Lee*

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

Methane (CH₄) is considered as one of the most important greenhouse gases owing to its 20-fold higher heat capacity compared with that of carbon dioxide (CO₂). Preliminary studies have aimed to elucidate the mechanisms of soluble methane monooxygenase (sMMO) involved in this extremely stable C–H activation (104.9 kcal/mol) through intermediate studies, advanced spectroscopies, and structural researches, mostly in *Methylosinus trichosporium* OB3b and *Methylococcus capsulatus* Bath, although mechanistic studies are still required. In this study, *M. sporium* 5 was cultured in a tightly regulated NMS media by supplying methane and air to understand its growth and the expression levels of multi-component enzymes. MMOH was found to be highly expressed in *M. sporium* 5, and it was purified to evaluate its catalytic activities using diverse substrates. MMOB and MMOR were also expressed in *E. coli* via constructed plasmids to obtain highly purified enzymes. The successfully expressed and purified enzymes were utilized to measure specific enzyme activities (SEA), and these results showed that *M. sporium* 5 exhibits optimal activity at pH 7.5. The electron transfer environment of MMOR is crucial for the activity of sMMO, and different acidities may change the electron transfer environment. The mutational studies of these reductase component proved that FAD binding residues are crucial to maintain the binding of cofactors including FADH and [2Fe-2S] cluster.

Poster Presentation : **INOR.P-93**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Structural roles of FAD-binding domain in reductase, MMOR, from *Methylosinus sporium 5*

Chae Min Lee, Yunha Hwang, Seung Jae Lee*

*Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University,
Korea*

The resting state of MMOH is reduced by the addition of electrons through MMOR and reduced di-iron active site ($\text{Fe}^{\text{II}}\text{-Fe}^{\text{II}}$) can activate molecular oxygen (O_2) for C-H activation. The essential intermediates from P*, H_{peroxo} , and Q can be generated by the O_2 activation from reduced MMOR, but the accurate electron-transfer pathways need to be further elucidated. MMOR has two cofactors including FAD/NADH-binding domain (MMOR-FAD) and [2Fe-2S] cluster to transfer electrons from NADH to di-iron active site housed in α -subunit MMOH. Although the structural information is available from solution nuclear magnetic resonance (NMR) of each domain, MMOR-FAD and MMOR-Fd, due to the size of molecule (39-kDa), the overall structure needs to be further discovered. The reductase component from *Methylosinus sporium 5* is successfully expressed and purified to understand biophysical aspects. The FAD content and ferrozine assay confirmed that presence of these cofactors and UV-vis spectra proved the presence of FAD (394 and 485 nm) and [2Fe-2S] cluster (332, 418, and 467 nm). The crystallization of MMOR provides structural insight of truncated version of MMOR-FAD binding domain generated by protease activity. The residues including S159, S160, Y161, and S184 generated hydrogen bonds with FAD with 2.5 – 3.5 Å apart. The mutated MMOR was successfully purified and confirmed the modification of iron contents and concentration of FAD. These results confirmed that the expression of reductase components affects the cofactor interactions of MMOR. In addition, the modification of MMOR-FAD affects the structural components of iron-sulfur clusters.

Poster Presentation : **INOR.P-94**

Inorganic Chemistry

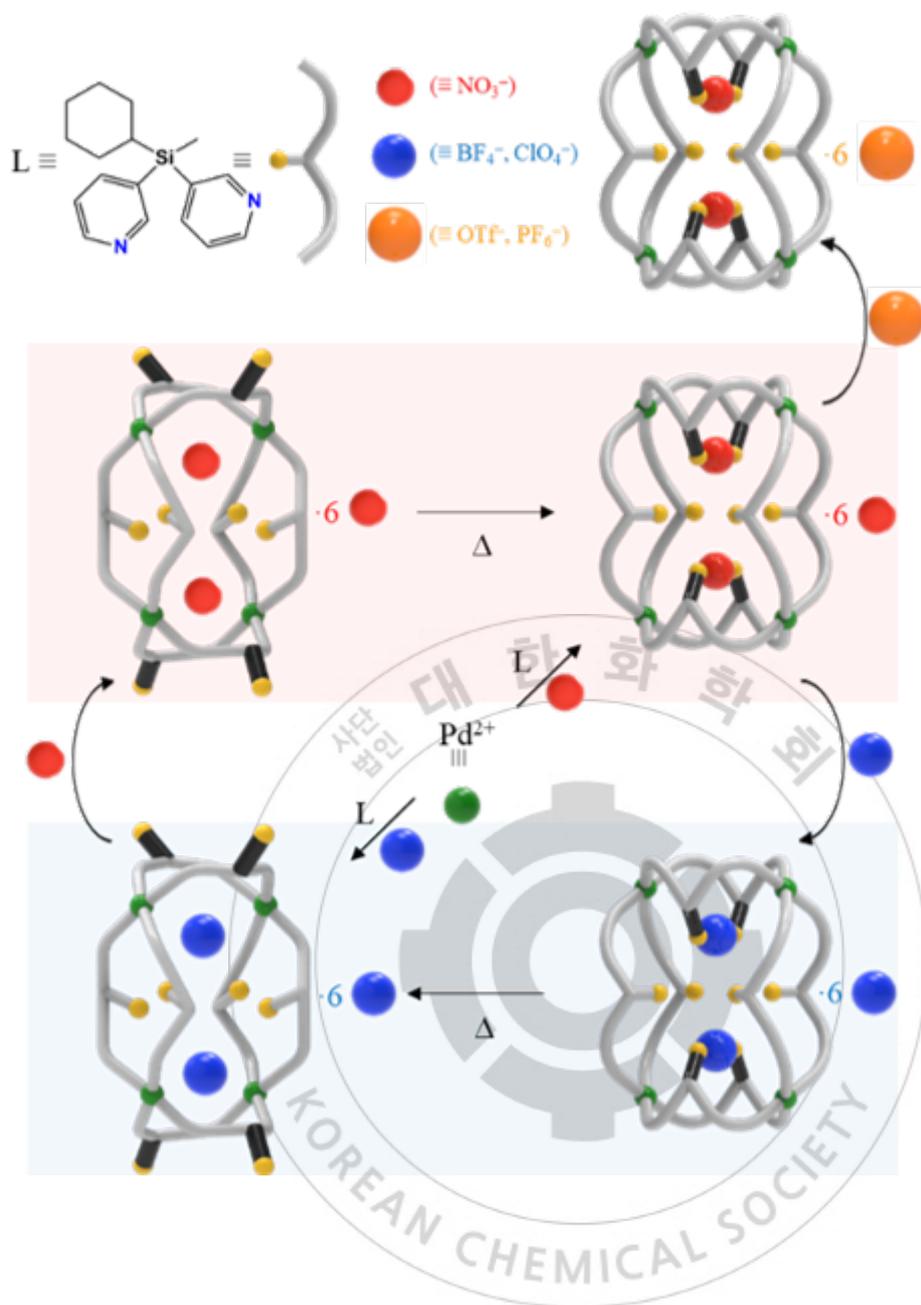
Zoom 3 FRI 15:00~16:00

A Cyclic Manipulation of Peanut Cage Isomers via Anion Exchange and Isomerism

Dongwon Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

A cyclic manipulation of peanut-cage isomers, *endo*-Me₈-[X₂@Pd₄L₈]X₆ and *exo*-Me₄,*endo*-Me₄->-[X₂@Pd₄L₈]X₆ (X⁻ = NO₃⁻, BF₄⁻, ClO₄⁻; L = cyclohexyl(methyl)-bis(3-pyridyl)silane), has been achieved via anion exchange and unusual cage isomerism. Anion exchange of the cage isomers preserves the integrity of the isomeric skeleton, and accordingly, pairs of peanut-cage isomers were efficiently constructed via both self-assembly and the anion exchange. The most momentous feature is that the cage isomers from the anion exchange isomerizes to its corresponding isomer in Me₂SO in the range of 80-90 °C, without any decomposition via an “expansion-rotation-contraction” mechanism. The cage system shows a contradictory behavior of “dynamic-but-tight cage” in solution.



Poster Presentation : **INOR.P-95**

Inorganic Chemistry

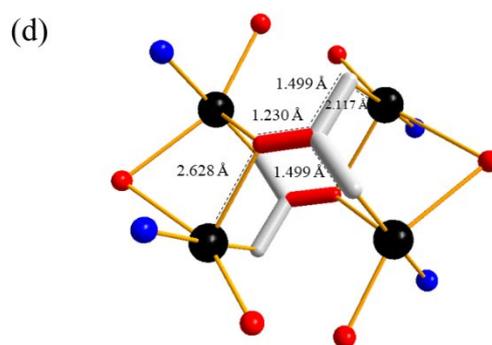
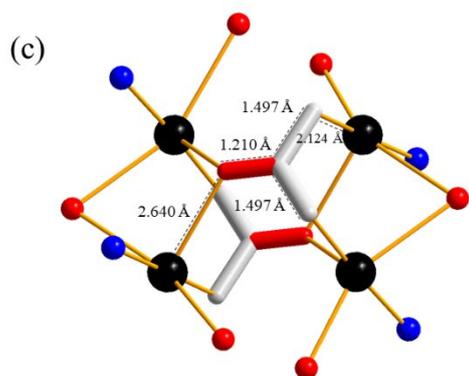
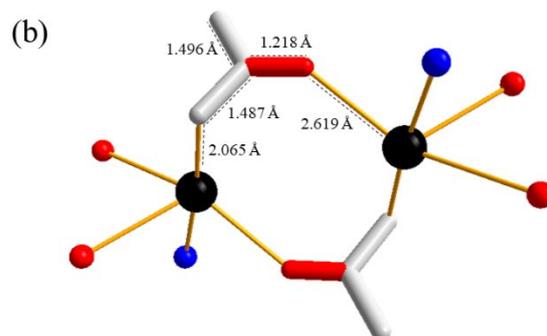
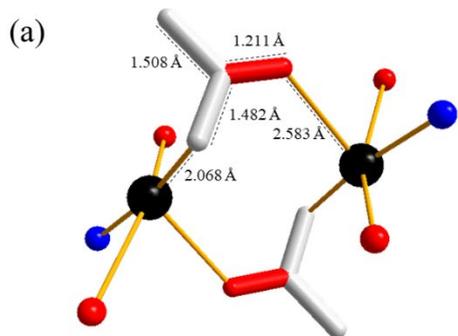
Zoom 3 FRI 15:00~16:00

Straightforward Formation of Acetyl Monoanion, Dianion as Synthons: Self-assembly of Mercury(II) with Pyridyl Donor Ligands in Acetone

Seok Kyun Jeong, 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 ($\text{CH}_3)_2\text{C}=\text{O}$ of acetone itself is in equilibrium with its enol isomer ($\text{CH}_3\text{C}(\text{OH})=\text{CH}_2$). 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 vigorous condition such as strong bases, lithium diisopropylamide (LDA). 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 acetyl dianion, all of which can exist in equilibrium simultaneously. To the best of our knowledge, no examples of the X-ray structure on acetyl coordination for mercury(II) complexes has been described at all. In this context, two crucial aims of the present research were to explore stable acetyl species via self-assembly of $\text{Hg}(\text{ClO}_4)_2$ with naphthalene-2,6-diylidipicolinate(L^1) or 1,3-bis(dimethyl(pyridin-3-yl)silyl)propane(L^2) in acetone under mild condition and to efficiently trap the acetyl dianion species in the supramolecular 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.



Poster Presentation : **INOR.P-96**

Inorganic Chemistry

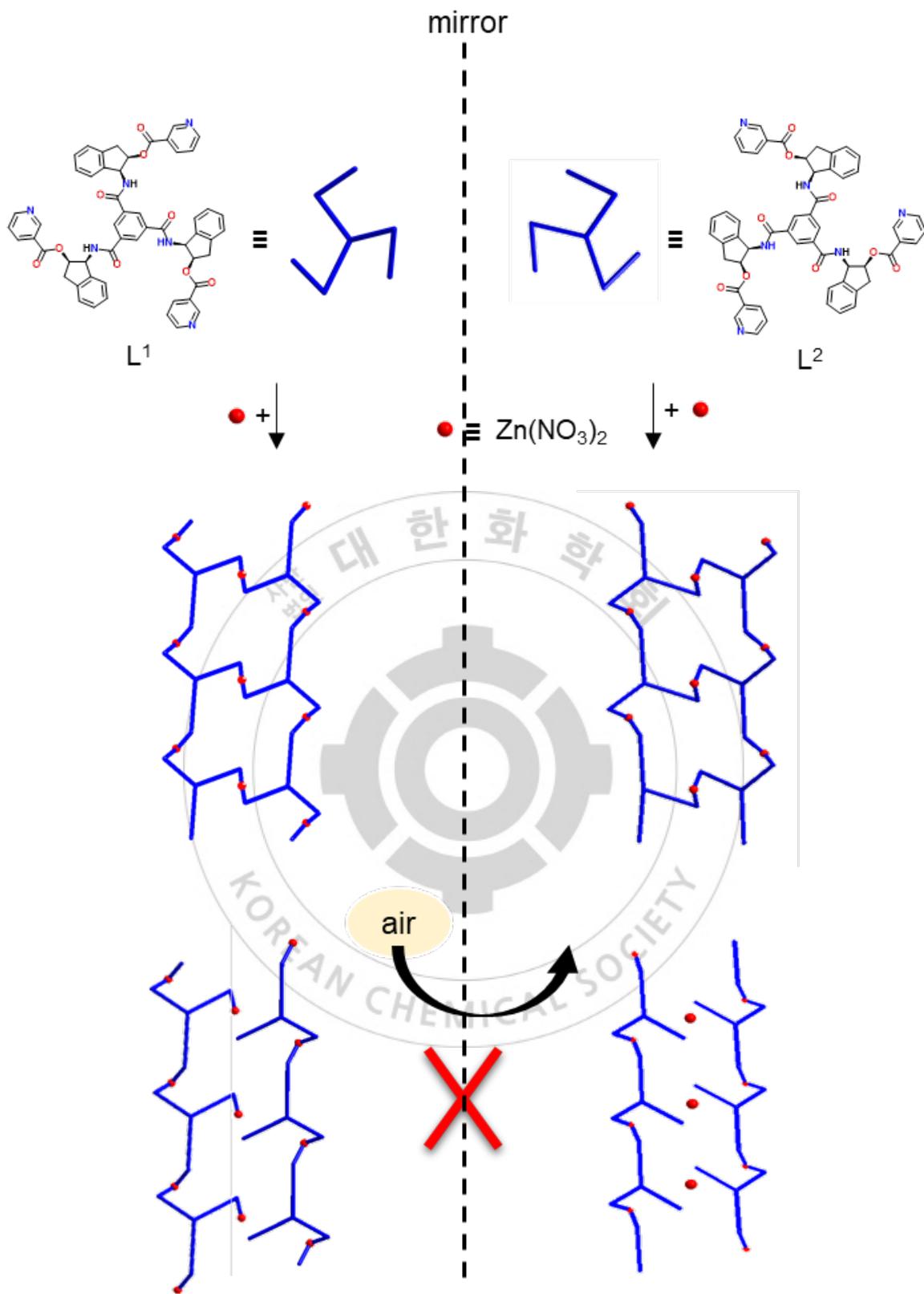
Zoom 3 FRI 15:00~16:00

Zn(II) complex using new chiral ligand (1*S*, 2*R*)-BTIT, (1*R*, 2*S*)-BTIT : Ladder foothold bisected by moisture

Junmyeong Park, Do Heon Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

New ligand (1*S*,1'*S*,1''*S*,2*R*,2'*R*,2''*R*)-(benzenetricarbonyltris(azanediyl))tris(2,3-dihydro-1*H*-indene-2,1-diyl) trinicotinate and (1*R*,1'*R*,1''*R*,2*S*,2'*S*,2''*S*)-benzenetricarbonyltris(azanediyl))tris(2,3-dihydro-1*H*-indene-2,1-diyl) trinicotinate are synthesized by (1*S*,2*R*)-(-)-*cis*-1-Amino-2-indanol and (1*R*,2*S*)-(+)-*cis*-1-Amino-2-indanol. Self-assembly of Zn(NO₃)₂ with L as a tridentate *N*-donor. It produces new 1D-ladder structures. The 1D-ladder has plywood packing by stacking 60 degrees staggered. The tridentate ligand has a three parts of coordination bond, two of which are depicted in a straight line to form the legs of the ladder, and one part is the foothold of the ladder. However, when a complex is exposed to moisture in the air, the H₂O forms new bonds with the zinc. Uniquely, at this time, only the bond that corresponds to the foothold of the ladder is broken. It is depicted that the ladder foothold is bisected. Curiously, this phenomenon occurs in different structures between enantiomers.



Poster Presentation : **INOR.P-97**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Modular interlayer distance via adsorption/desorption of cyclic hydrocarbons in SCSC mode

Junhee Kim, Ok-Sang Jung*

Department of Chemistry, Pusan National University, Korea

Self-assembly of Cadmium(II) nitrate tetrahydrate with a new C_2 -symmetric multidentate *N*-donor ligand gives rise to crystals of two-dimensional (2D) frameworks (sql), with available interlayer open space occupied by solvate 1,4-dioxane molecules. The interlayer distance between the 2D frameworks can be modulated via adsorption/desorption of various cyclic hydrocarbons in the single-crystal-to-single-crystal (SCSC) mode. In this mode, the 1,4-dioxane solvate molecules were replaced for adsorption of benzene, 1,4-dioxane, anisole, *trans*-decalin, 1,4-benzodioxane, and 1,5-cyclooctadiene. The overall serve to exemplify the control of the van der Waals interlayer interaction in 2D sheets, which control can delicately affect task-specific functions according to the interlayer distance.

Poster Presentation : **INOR.P-98**

Inorganic Chemistry

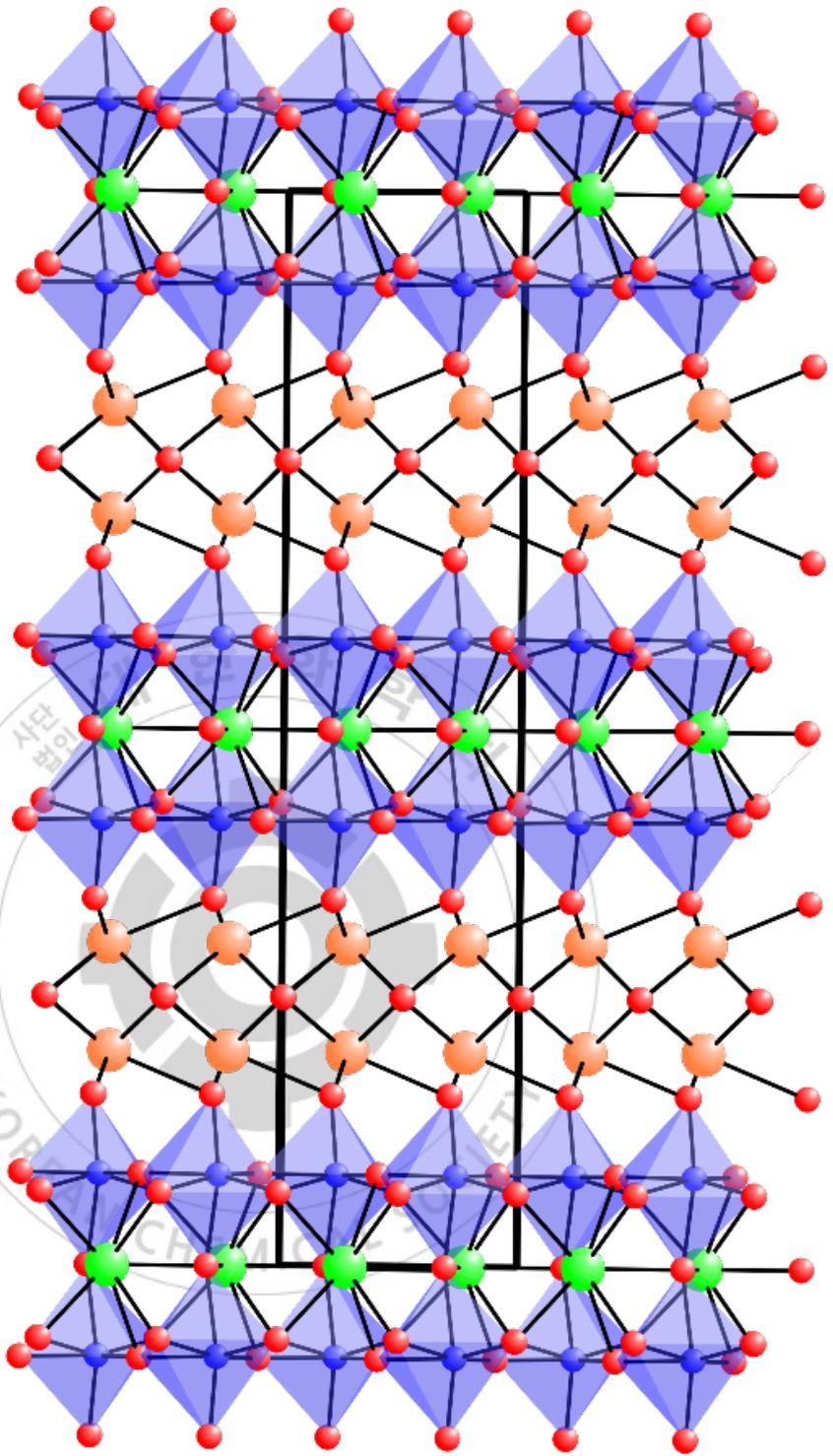
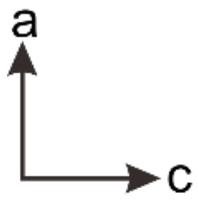
Zoom 3 FRI 15:00~16:00

Crystal structure and nonlinear optical property of a rare earth-doped Aurivillius-type perovskite

Kisung Kim, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Perovskite has been widely studied with great interest for its multifunctionality and wide industrial applications. Phase transition and other electrical properties such as ferroelectricity and piezoelectricity of one of the Aurivillius-type polar perovskites with noncentrosymmetric structure, $\text{Na}_{0.5}\text{Bi}_{2.5}\text{Nb}_2\text{O}_9$, has been studied. Since the material contains second-order Jahn–Teller distortive cations, Bi^{3+} and Nb^{5+} , we have explored other interesting optical properties by substituting lone pair cations with lanthanide elements. Crystal structure for $\text{Na}_{0.5}\text{Bi}_{2.5}\text{Nb}_2\text{O}_9$ was also redetermined by single crystal X-ray diffraction to better explain the origin of the nonlinear optical properties. The doped rare earth cations were confirmed to occupy only the Bi(2) site (8b site, i.e., B site) and are disordered with Bi^{3+} cations.



- BiNa
- Nb
- Bi
- O

Poster Presentation : **INOR.P-99**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Synthesis and characterization of new chiral zinc-coordination polymers

Joonhyuk Kee, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Metal-organic coordination polymers (MOCP) reveal many interesting properties such as gas storage, ion conductivity, and ion exchange. In this research, we have synthesized a novel chiral organic ligand and introduced it to new zinc-coordination polymers. The title compounds crystallized in the orthorhombic chiral space group, $C222_1$ with chiral organic ligands and 4-coordinate Zn^{2+} cations. Second-harmonic generation (SHG) measurements indicate that the title compounds have large SHG efficiency of *ca.* 4.5 times that of KH_2PO_4 and phase-matching behavior because of the large hyperpolarizability of the ligands. Infrared spectra show vibrations occurring from the organic ligands Zn–O bonds in the title compounds. UV-vis diffuse reflectance indicates that the title compounds have band gap of *ca.* 4.15 eV. Solid-state circular dichroism (CD) confirms the chirality of the title compounds by the positive and negative CD signals.

Poster Presentation : **INOR.P-100**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Lewis-Base Characteristics of Chloroform and Its Coordination Ability at Metal Center of Paddlewheel Metal-Organic Framework

Sun Ho Park, Nak Cheon Jeong^{1,*}

Department of 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), a subset of crystalline porous materials that consist of metal ions (or metal-oxo clusters) and multitopic organic linkers, have shown critical potentials in various applications. In particular, MOFs with open coordination sites (OCSs), where Lewis-base guest molecules can be bound with coordination bonds, often function vital role in potential applications such as catalysis, gas absorption, gas separation, drug delivery, chemical sensing, electronics, and ionic conduction. Although the OCSs are a substantial factor in such applications, what Lewis-base guest molecules and how those molecules can form coordination bondings at the OCSs are still a challenging issue. Meanwhile, equilibrium processes in chemical reactions has been extensively studied in contemporary chemistry because the control of the chemical reaction has been considered as the most important one in academia as well as industry. However, coordinative equilibrium in MOFs have been rarely studied. In this presentation, we show the ability of chemically inert “chloroform” in its coordination bond formation and coordination bond exchange. Further, we demonstrate that the coordination exchange ability of the chloroform performs “coordinative equilibrium” via its exchange of strong Lewis-base molecules such as H₂O, MeOH, EtOH, and DMF. The demonstration was performed through real-time in situ NMR and Raman studies. On the basis of these studies, we prove that chloroform can play a role as a weak Lewis-base molecule with lone-paired electrons at its chlorine atom.

Poster Presentation : **INOR.P-101**

Inorganic Chemistry

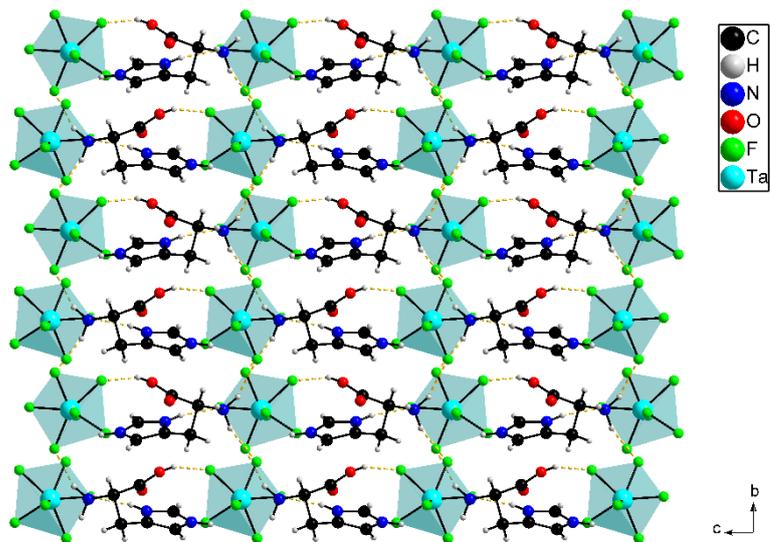
Zoom 3 FRI 15:00~16:00

Synthesis and characterization of enantiopure histidinium-driven noncentrosymmetric chiral tantalum fluorides

Heejung Choi, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Enantiopure histidinium-driven noncentrosymmetric chiral tantalum fluorides were successfully synthesized by a slow evaporation method. The structure of title compounds crystallizing in the polar space group, $P2_1$, consists of L- or D-histidinium cations and distorted mono-capped trigonal prismatic polyhedra of tantalum fluorides. Infrared spectra reveal Ta–F stretching vibrations at 550–510 cm^{-1} , which confirm the existence of Ta–F bonds in the reported compounds. Partial density of states for the title compounds indicate that C atoms of histidinium mainly contribute to the conduction band and valence band. Ultraviolet-visible diffuse reflectance spectra of the title compounds show a strong band at *ca.* 240 nm. Opposite signals found in circular dichroism spectra of the reported compounds confirm the chiralities of enantiomorphs. Second harmonic generation (SHG) measurements suggest that the reported compounds have an SHG efficiency of about 10 times that of $\alpha\text{-SiO}_2$.



Poster Presentation : **INOR.P-102**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Reversible Transformation between Interpenetrated MOF-14 and Non-interpenetrated MOF-143

Cheol Yeong Heo, Nak Cheon Jeong*

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

Metal-organic frameworks (MOFs), a subset of crystalline porous materials that consist of metal ions (or metal-oxo clusters) and multitopic organic linkers, have extensively studied since the MOFs have shown their potential functions in various applications such as catalysis, gas absorption, gas separation, drug delivery, chemical sensing, electronics, and ionic conduction. Although MOFs should possess large open cages with permanent porosities for such application, several MOFs with large open cages such as MOF-143 often function negatively by the double interpenetration of their frameworks, leading to the block of large open pores and thereby, reducing their porosities. So far, the control of interpenetration in MOFs has been intensively studied because while non-interpenetrated MOFs can be utilized positively for such wide applications, interpenetrated MOFs can be limited in such application despite their high thermodynamic stabilities. Thus, most research has been driven to serendipitously synthesize or rationally design non-interpenetrated MOFs from born. Meanwhile, post-synthetic transformation of interpenetrated MOFs can be an excellent strategy to form non-interpenetrated MOFs. 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 performed through the exchange of protic solvents at room temperature, whereas the reverse transformation was conducted in the presence of pyridine and DMF at 100 °C. We believe that our observation and demonstration can aid in understanding the assembly and disassembly nature of framework.

Poster Presentation : **INOR.P-103**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

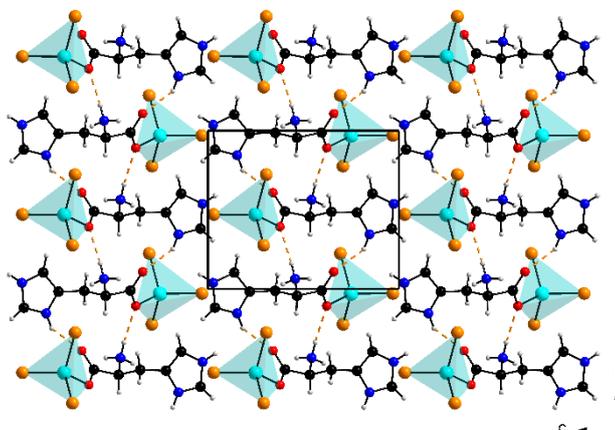
Synthesis, Structure, and Characterization of Chiral Zinc Coordination Compounds

Woo Young Seo, Kang Min Ok^{1,*}

chemistry, Sogang University, Korea

¹*Department of Chemistry, Sogang University, Korea*

Two new chiral zinc coordination compounds were successfully synthesized by a slow evaporation method. Single crystal X-ray diffraction shows that the reported compounds crystallize in the polar monoclinic space group, $P2_1$. The Zn atom is connected to three Br atoms and one O atom, forming a distorted $ZnBr_3O$ tetrahedra. Powder X-ray diffraction confirm that the reported compounds were synthesized in phase pure forms. Thermogravimetric analysis data indicate that the reported compounds are thermally stable up to *ca.* 230 °C. Ultraviolet-visible diffuse reflectance spectra indicate that the compounds have approximate band gaps of *ca.* 5.02 eV. Powder second-harmonic generation (SHG) measurements indicate that the reported compounds have SHG efficiencies of *ca.* 5 times that of α - SiO_2 .



Poster Presentation : **INOR.P-104**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Preparation and Properties of 1,1-Dialkyl-2,5-bis(trimethylsilylethynyl)-3,4-diphenyl-siloles

Se yeon Park, Young Tae Park*, Ji Hun Lee

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 1,1-dialkyl(ethyl, or *iso*-propyl, or *n*-hexyl)-bis(phenylethynyl)silanes with lithium naphthalenide, ZnCl₂, and *N*-bromosuccinimide (NBS). 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. The crude products were purified using recrystallization in hexane as solvent. The obtained materials are soluble in usual organic solvents such as DCM and THF. Photochemical properties of the prepared materials were investigated with UV-Vis absorption, excitation, and fluorescence emission spectroscopy. The electrochemical properties of the synthetic materials related to lithium-ion batteries was also studied. Acknowledgment. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education of the Republic of Korea (NRF-2020R111A3A04036901).

Poster Presentation : **INOR.P-105**

Inorganic Chemistry

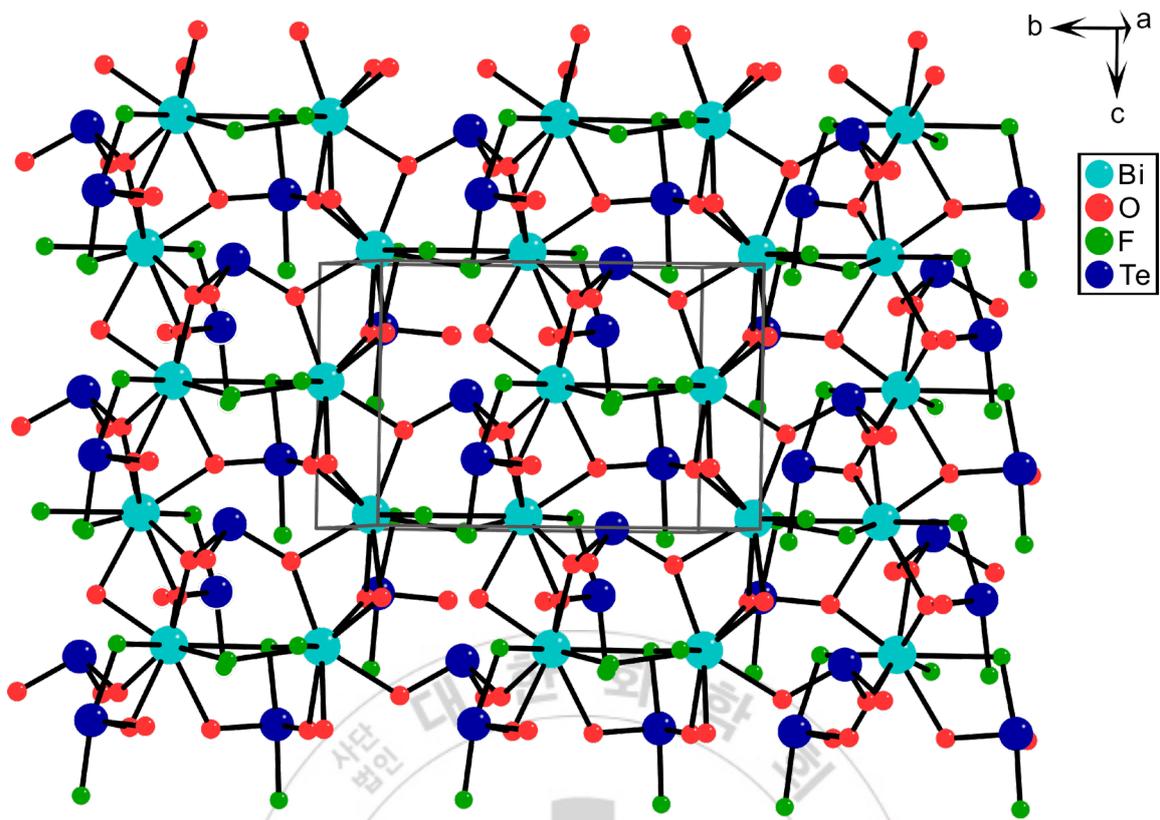
Zoom 3 FRI 15:00~16:00

Hydrothermal Synthesis, Structure Determination, and Characterization of a Bismuth Tellurite Fluoride

Jee Yoon Chung, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

A novel bismuth tellurite fluoride, $\text{Bi}_3(\text{TeO}_3)(\text{TeO}_2\text{F}_2)_3$ (1), has been synthesized through a hydrothermal reaction by using Bi_2O_3 , TeO_2 , and HF as reagents. Single crystals of compound 1 were grown with a mineralizer, nitric acid. Single crystal X-ray diffraction suggests that the title compound crystallizes in the polar space group, $P6_3mc$ with a three-dimensional structure composed of BiO_6F_3 , TeO_3 , and TeO_2F_2 groups. Based on the ultraviolet-visible diffuse reflectance spectrum, the band gap of the material was calculated to be 3.85 eV using the Kubelka–Munk function. Infrared spectrum reveals peaks occurring from Bi–O/F, Te–O, and Te–F vibrations in the range of 400–500, 550–750, and 750–825 cm^{-1} , respectively. Thermal analysis shows that the title compound is thermally stable up to 250 °C and decomposes to $\text{Bi}_{0.5}\text{Te}_{0.5}\text{O}_2$ upon further heating to 600 °C. Second-harmonic generation (SHG) measurements indicate that compound 1 is phase-matchable and has an SHG efficiency of 1.4 times that of KH_2PO_4 (KDP).



Poster Presentation : **INOR.P-106**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

An Investigation of Collisional Electron-Injection Process in Semi-Heterogeneous Photocatalytic System (Porphyrin Dye + TiO₂/Re(I)) for CO₂ Reduction.

Yunjeong Seo, Daehan Lee, Sanghun Lee¹, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son^{*}

Department of Advanced Materials Chemistry, Korea University, Korea

¹*Department of Advanced Materials Chemistry, Korea University Sejong Campus, Korea*

We report a collisional electron-injection process in the semi-hetero hybrid photocatalytic system consisting of non-anchored porphyrins and TiO₂/Re(I) nanoparticles. The net hetero-collisional electron transfer from the non-anchored fluorescent porphyrin sensitizer to the TiO₂ catalytic particles was a major event during the initial stage of the catalysis. According to in situ UV-vis absorption spectroscopy and mass analysis of dye solution filtered after photolysis, the initially added porphyrin dye is found to experience a photomodification accompanied by a breakage of π -conjugation and loss of the bulky substituents. With the structural identification of deformed porphyrin species, two acetyl- or ethyl-group modified porphyrins were prepared, respectively referred to as **ZnP_{Acet}** and **ZnP_{Et}**, and this modification elevated the corresponding excited-state energy levels when comparing **ZnP** with **ZnP_{Et}**, consequently shortening the activity delay at the early stage of photolysis. Thus, chemical modification had a favorable effect on the photosensitizing and electron transportation abilities of the dye. The high activation barrier for the collisional electron transfer process, as estimated from the Arrhenius plot of the temperature-dependent quenching rate, supports that the net efficiency of electron transport to TiO₂ is sensitively affected by the small difference in the reduction potential (E_{red}) of porphyrin dye.

Poster Presentation : **INOR.P-107**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

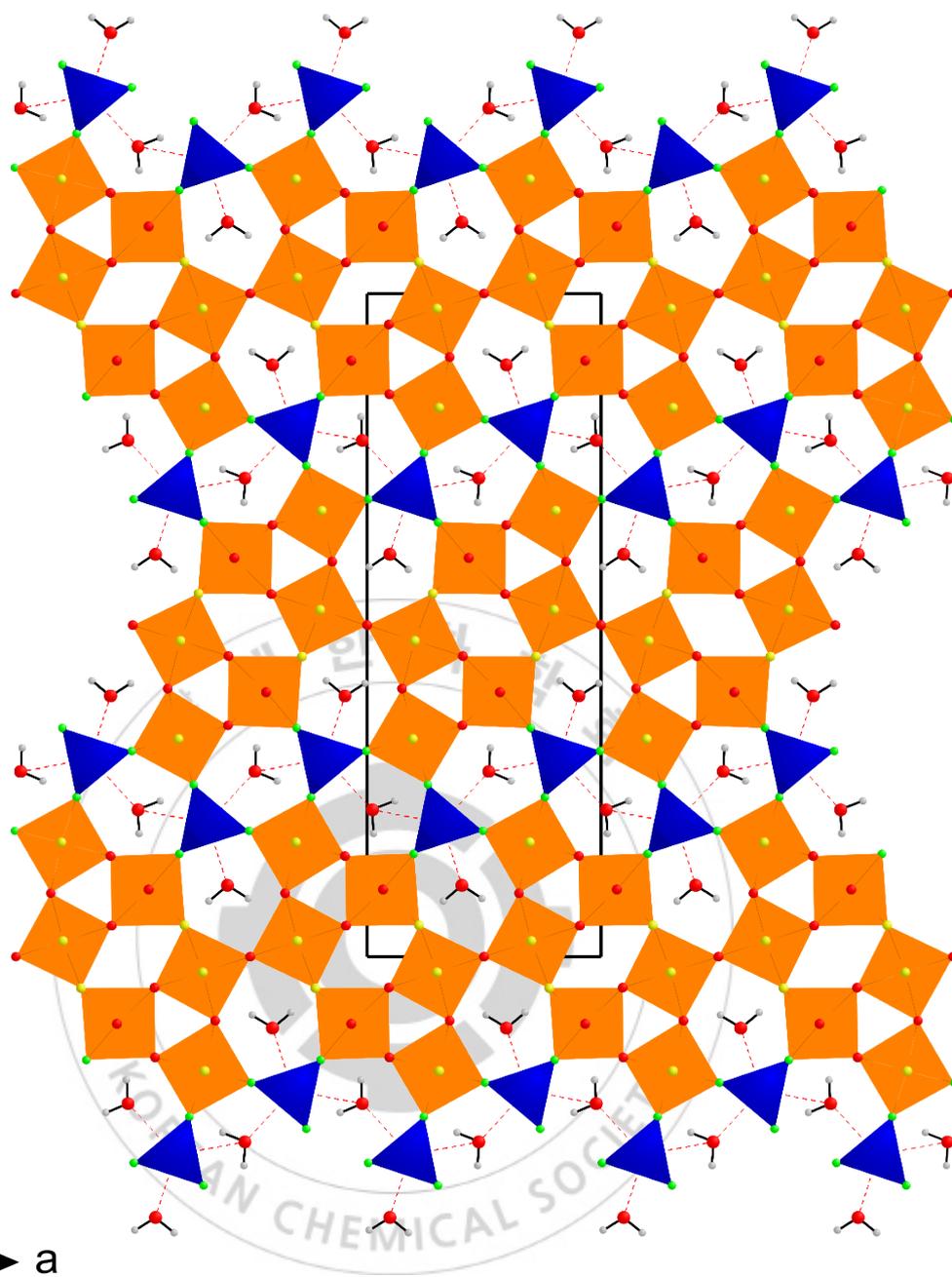
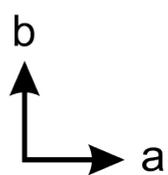
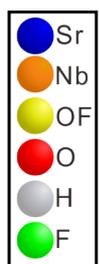
Sr₂Nb₆O₁₃F₈·4H₂O: A new strontium niobium oxyfluoride with a three-dimensional tungsten bronze-type structure

Euna Ko, Kang Min Ok^{1,*}

Chemistry, Sogang University, Korea

¹*Department of Chemistry, Sogang University, Korea*

A new strontium niobium oxyfluoride with a three-dimensional (3D) tungsten bronze-type structure, Sr₂Nb₆O₁₃F₈·4H₂O (1) has been synthesized via a hydrothermal reaction. Single crystal X-ray diffraction indicates that the title compound crystallizes in the centrosymmetric orthorhombic space group, *Pbam* (No.55). Compound 1 features a three-dimensional structure composed of Nb(1)O₂F₂(O/F)₂, Nb(2)O₄F(O/F), Nb(3)O₃(O/F)₃ octahedra, SrO₃F₆ tricapped trigonal prism, and water molecules. The niobium oxyfluoride octahedra share corners through O and O/F atoms to form a Nb₃O₆F₃(O/F)₆ ring along the *c*-axis. The 3D structure of compound 1 is comprised of three-, four-, and five-membered rings (5-MRs), which is a new variant of tetragonal tungsten bronze geometry. A more detailed structural analysis reveals that water molecules reside in the 5-MR channels. Thermal analysis indicates that compound 1 is thermally stable up to 250 °C. The infrared analysis shows that the title compound has Nb–O, Nb–F, Nb–O/F–Nb, and O–H bond. UV-visible diffuse reflectance spectrum reveals that compound 1 has the optical band gap of 3.22 eV. The partial density of states of compound 1 indicate that the valence band maximum mainly consists of O-2p and F-2p states, whereas the conduction band minimum is dominated by Nb-4d.



Poster Presentation : **INOR.P-108**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

SuFExable Metal-Organic Frameworks with Benign Transition Metals

Seungjae Park, Eunsung Lee*

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

Metal-organic frameworks (MOFs) are representative robust and porous crystalline materials consisting of metals and organic linkers. In the past few decades, numerous metal-organic frameworks (MOFs) and their synthetic methods have been reported to develop their interesting applications. Among various methods, post-synthetic modification (PSM) strategies have been mainly utilized to introduce novel properties in the MOFs.¹ The first option to introduce the property is to modify the organic linkers. Recently, a new type of PSM strategy utilizing sulfur(VI) fluoride exchange (SuFEx),² was reported.³ With this method, several functional groups were successfully substituted with high yields. Here we report two new MOFs with sulfonyl fluoride that is possible for PSM via SuFEx. Two new MOFs are prepared with benign metals (Cu and Zn). They are expected to have low toxicity and competitive price. They are successfully characterized by SXRD, PXRD, and gas sorption. Currently, the applications using these materials are in development. Reference[1] Cohen, S. M., J. Am. Chem. Soc., 2017, 139, 2855.[2] Dong, J.; Krasnova, L.; Finn, M. G.; Sharpless, K. B. Angew. Chem Int. Ed., 2014, 53, 9430.[3] Park, S.; Song, H; Lee, E. et al ACS Appl. Mater. Interaces, 2018, 10, 33785.

Poster Presentation : **INOR.P-109**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Cobalt(II) Complexes Containing *N,N*-bis((3,5-dimethyl-1H-pyrazol-1-yl)methyl)amines: Synthesis, structural characterization and application to polymerization of methyl methacrylate

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We have synthesized series of Co(II) complexes with ligands **L_A**, **L_B** and **L_C** where **L_A** is 1-cyclohexyl-*N,N*-bis((3,5-dimethyl-1*H*-pyrazol-1-yl)methyl)methanamine, **L_B** is 1-(3,5-dimethyl-1*H*-pyrazol-1-yl)-*N*-((3,5-dimethyl-1*H*-pyrazol-1-yl)methyl)-*N*-(furan-2-ylmethyl)methanamine and **L_C** is 4-isopropyl-*N,N*-bis((3,5-dimethyl-1*H*-pyrazol-1-yl)methyl)benzenamine. All complexes were characterized by ¹H-NMR, ¹³C-NMR, IR, and elemental analyzer. In addition, the molecular structures of these complexes were characterized by X-ray single crystal diffraction. The catalytic properties of these complexes toward the polymerization of methyl methacrylate (MMA) in the presence of MMAO by of all complexes was investigated at 60 °C.

Poster Presentation : **INOR.P-110**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Polymerization of Cyclic Olefin by Precatalyst Cobalt(II) Complexes

Jawon Jang, Hyosun Lee^{1,*}

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

The reaction of **[CoCl₂·6H₂O]** with *N*-substituted *N,N*-bis((1*H*-pyrazol-1-yl)methyl)benzenamine ligands ($L_n = L_A - L_D$) where L_A is *N,N*-bis((1*H*-pyrazol-1-yl)methyl)cyclohexanamine, L_B is *N,N*-bis((1*H*-pyrazol-1-yl)methyl)-1-phenylethanamine, L_C is *N,N*-bis((1*H*-pyrazol-1-yl)methyl)-1-(furan-2-yl)methanamine and L_D is 4-isopropyl-*N,N*-bis((1*H*-pyrazol-1-yl)methyl)benzenamine, gave Co(II) complexes $[L_nCoCl_2]$, respectively. All complexes were characterized by ¹H-NMR, ¹³C-NMR, IR, and elemental analyzer. The molecular structures of Co(II) complexes were characterized by X-ray single crystal diffraction. The catalytic properties of these complexes toward the polymerization of norbornene (NB) and 5-norbornene-2-carboxylic acid (MeNB) in the presence of MMAO by of all complexes was investigated at 90 °C.

Poster Presentation : **INOR.P-111**

Inorganic Chemistry

Zoom 3 FRI 15:00~16:00

Cobalt(II) and palladium(II) complexes with (*E*)-3-methoxy-*N*-(quinolin-2-ylmethylene)propan-1-amine: Synthesis, structure and polymerization of norbornene

Kyeonghun Kim, Hyosun Lee^{1,*}

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

We have synthesized Co(II) and Pd(II) complexes supported by ligand (*E*)-3-methoxy-*N*-(quinolin-2-ylmethylene)propan-1-amine (L_{QM}). Both complexes, $[L_{QM}CoCl_2]$ and $[L_{QM}PdCl_2]$ were characterized by 1H -NMR, ^{13}C -NMR, IR, elemental analyzer and single crystal X-ray diffraction. Specifically, $[L_{QM}CoCl_2]$ and $[L_{QM}PdCl_2]$ adopted distorted trigonal bipyramidal and square planar geometry, respectively. The catalytic properties of these complexes toward the polymerization of norbornene (NBE) in the presence of modified methylaluminoxane (MMAO) were also investigated.

Poster Presentation : **INOR.P-112**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Benzoxadiazole-based Fluorescent Probe for Hydrogen Sulfide Detection in Mitochondria: Cancer Cell-Specificity

Jinheung Kim

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

This work describes the design and biological applications of a novel colorimetric and fluorescence turn-on probe for hydrosulfide detection. The probe was designed to introduce hemicyanine as the fluorescent skeleton and 7-nitro-1,2,3-benzoxadiazole as the recognition site. The optical properties and responses of the probe towards HS⁻, anions, and some biothiols indicate an impressively high selectivity of the probe towards HS⁻ such that it can be effectively used as an indicator for monitoring the level of HS⁻ in living cells. In biological experiments using the probe, the H₂S levels are found to be higher in cancer cells than in normal cells. In addition, the probe is shown to specifically and rapidly detect endogenous H₂S which is produced primarily in the mitochondria of cancer cells, as demonstrated by a co-localization experiment using specific trackers for the detection of cellular organelles in pharmacological inhibition or stimulation studies, without any significant cytotoxic effects. Thus, the results of chemical and biological experiments described herein demonstrate the potential of this novel probe to specifically, safely, and rapidly detect H₂S to distinguish cancer cells from normal cells by targeting it specifically in mitochondria.

Poster Presentation : **INOR.P-113**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Efficient and Selective Photocatalytic Conversion of CO₂ by New Nickel Complexes

Jinheung Kim^{*}, Sung-Jin Kim¹, Byeongmoon Jeong², Youngmee Kim²

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

¹Department of Chemistry, Ewha Womans University, Korea

²Department of Chemistry and Nano Science, Ewha Womans University, Korea

Artificial photosynthesis using earth-abundant metal complexes has recently great attention in relation with renewable energy. Mononuclear 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 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-114**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Photochemical CO₂ Conversion Catalyzed by Half-Metallocene Ir(III) Catalyst: Highly Efficient CO₂-to-CO/Formate Conversion and Its Mechanistic Investigation

Daehan Lee, Yunjeong Seo, Sanghun Lee, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

This study details the photocatalytic CO₂-to-CO or formate conversion activities of two different photocatalytic systems (IrPS + Cp*IrPE and IrPS/TiO₂/Cp*IrP) to evaluate the catalytic behavior of homogeneous and heterogenized Cp*Ir(III) catalyst, respectively. A single run photolysis of the mixed homogeneous system (IrPS + Cp*IrPE) in the presence of 3 vol % water exhibited a maximal turnover number (TON) of ~800 for 48 h with a high product selectivity of formate (>97%), while the ternary hybrid system with TiO₂-immobilized Cp*IrP showed the relatively lower but steady CO₂-to-CO and CO₂-to-formate conversion activities (a TON of >560 for 100 h), reflecting the CO₂ reduction route bisected by heterogenization of Cp*IrP. The mechanistic investigations along with photophysical and electrochemical studies suggests that the occurrence of MLCT ($[\text{Cp}^*\text{Ir}^{\text{II}}(\text{bpy})]^+ \rightarrow [\text{Cp}^*\text{Ir}^{\text{III}}(\text{bpy}^{-\cdot})]^+$) onto the electron-withdrawing n-type TiO₂ opens catalytic route toward Cp*Ir^{III}-COOH intermediate that results in CO₂-to-CO conversion, apart from the typical catalytic route via Cp*Ir^{III}-H intermediate for formate production.

Poster Presentation : **INOR.P-115**

Inorganic Chemistry

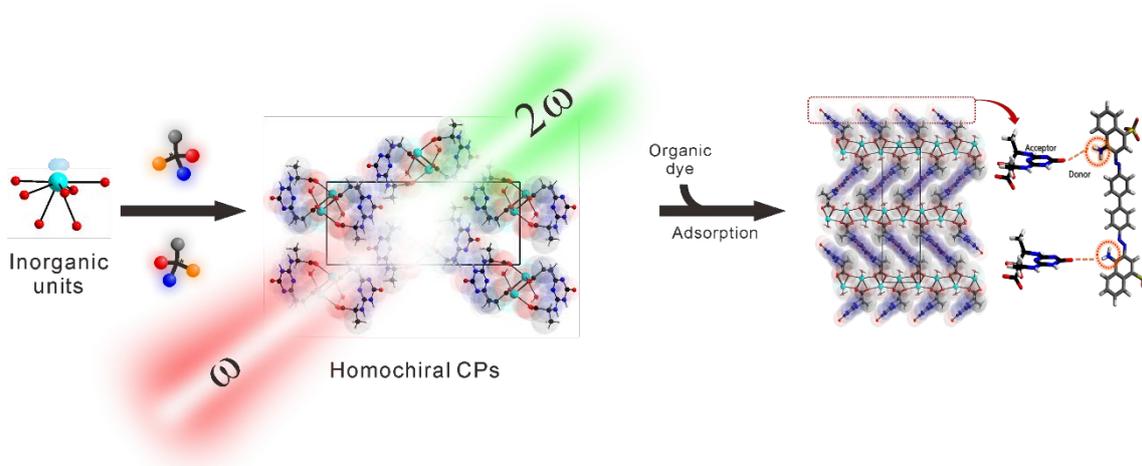
Zoom 3 FRI 16:00~17:00

Homochiral Pb-Coordination Polymers Constructed by Chiral Ligands: Nonlinear Optical Properties and Selective Dye adsorptions

Yunseung Kuk, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

Discovering novel multifunctional coordination polymers (CPs) composed of metal units and organic ligands have been of great interest owing to their potential applications such as catalyst, gas storage, separation, *etc.* Especially, a rational design of CPs can induce a variety of related useful properties such as catalytic activities with open metal sites, adjustable pore sizes, and host-guest interactions. In this research, we have synthesized homochiral CPs, *i.e.*, $[\text{Pb}(\text{R,R-TBA})(\text{H}_2\text{O})]\cdot 1.7\text{H}_2\text{O}$ (**R1**) and $[\text{Pb}(\text{S,S-TBA})(\text{H}_2\text{O})]\cdot 1.7\text{H}_2\text{O}$ (**S1**) ($\text{TBA} = 1,3,5\text{-triazine-}2(1H)\text{-one-}4,6\text{-bis(alanyl)}$), with the aid of designed chiral ligands. Compounds **R1** and **S1** crystallizing in the chiral space group, $P2_12_12_1$ (No, 19), reveal high water and chemical stabilities in a wide pH range. Furthermore, the title compounds not only exhibit second-harmonic generation signals originating from the macroscopic noncentrosymmetric structures, but also reveal a selective adsorption of anionic organic dyes *via* host-guest hydrogen bonding interactions. A detailed adsorption study of the title compounds towards a complete removal of organic dyes and the effect of pH and particle size on the adsorption are further discussed.



Poster Presentation : **INOR.P-116**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Photosensitization Behavior of P3HT Conjugated Polymer in Highly Durable CO₂ Reduction by Re(I)-Catalyst-Immobilized TiO₂ Hybrid Photocatalyst

Min Su Choe, Daehan Lee, Yunjeong Seo, Chul Hoon Kim, Sang Ook Kang, Ho-Jin Son*

Department of Advanced Materials Chemistry, Korea University, Korea

Herein, we report a detailed investigation of efficient hybrid photocatalyst system for carbon dioxide reduction. The system is based on a co-assembly of conjugated polymer photosensitizer (**P3HT**) and molecular Re(I) reduction catalyst on TiO₂ semiconductor. The hybrid system consists of **P3HT** (poly(3-hexylthiophene-2,5-diyl)) as a visible-light photosensitizer and *fac*-[Re(4,4'-bis(methylphosphonic acid)-2,2'-bipyridine)(CO)₃Cl] as a CO₂ reduction catalyst. The **P3HT** photosensitizer is coated onto Re(I) catalyst (ReP)-loaded TiO₂ particles to build up a new polymer-sensitized TiO₂ photocatalyst system (**P3HT**/TiO₂/ReP). The **P3HT**-based hybrid system showed the most durable catalytic activities compared to our previous ternary systems using molecular photosensitizer. Under irradiation with low energy light (>500 nm), the hybrid **P3HT**/TiO₂/ReP catalyst showed a TON of ~5300 over an extended time period of 830 h.

Poster Presentation : **INOR.P-117**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Highly Stable Sn(II)-based Two-Dimensional Organic–Inorganic Hybrid Perovskites Based on Stilbene Derivatives

In-Hyeok Park^{*}, Kian Ping Loh^{1,*}

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

¹*Department of Chemistry, National University of Singapore, Singapore*

Hybrid organic-inorganic perovskites have recently emerged as potential disruptive photovoltaic technology. However, the toxicity of lead used in state-of-the-art hybrid perovskites solar cell prevents large scale commercialization, thus it is necessary to develop lead-free alternatives. Sn-based perovskites are possible alternatives but are disadvantaged by its lack of stability in ambient air. Here, we report air stable Sn-based two-dimensional (2D) hybrid organic-inorganic perovskites, [(FSA)₂(MA)_(n-1)Sn_nI_(3n+1)] (*n* = 1 and 2; methylammonium iodide = MAI) using bulky stilbene derivatives as the organic cations (2-(4-(3-fluoro)stilbenyl)ethan ammonium iodide = FSAI).^[1] The air stability of the [(FSA)₂SnI₄] perovskites is attributed to the hydrophobic properties of fluorine-functionalized organic chains (FSA), as well as the strong cohesive bonding in the organic chains provided by H-bonds, CH₂···X type H-bonds, weak interlayer F···F interaction, and weak face-to-face type π-π interactions. Field effect transistor fabricated on exfoliated single crystal flake of [(FSA)₂SnI₄] exhibited a mobility of 0.023 cm²/Vs, and fast and stable photoconductor response. The details will be presented at the conference.

REFERENCE

[1] I.-H. Park, L. Chu, K. Leng, Y. F. Choy, W. Liu, I. Abdelwahab, Z. Zhu, Z. Ma, W. Chen, Q.-H. Xu, G. Eda, K. P. Loh, *Adv. Func. Mater.* **2019**, *29*, 1904810.

Poster Presentation : **INOR.P-118**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Investigation of morphology control in silver nanoparticle

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*Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University,
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Silver nanoparticles have shown unique optical properties from localized surface plasmon resonance (LSPR). Their LSPR bands can be fine-tuned by changing particle shape, size and composition, which ranges from 300 nm to 1200 nm. This tunability makes silver nanoparticles useful for optical sensing and bioimaging applications. We investigate seed-mediated silver nanoparticle growth to improve control of the silver nanoparticle morphology and uniformity. It is found that different seed shape and size have significant impact on the silver shell growth and following optical properties. Our examination will help develop a rational design rule to obtain optimal morphology of the silver nanoparticle for desired applications.

Poster Presentation : **INOR.P-119**

Inorganic Chemistry

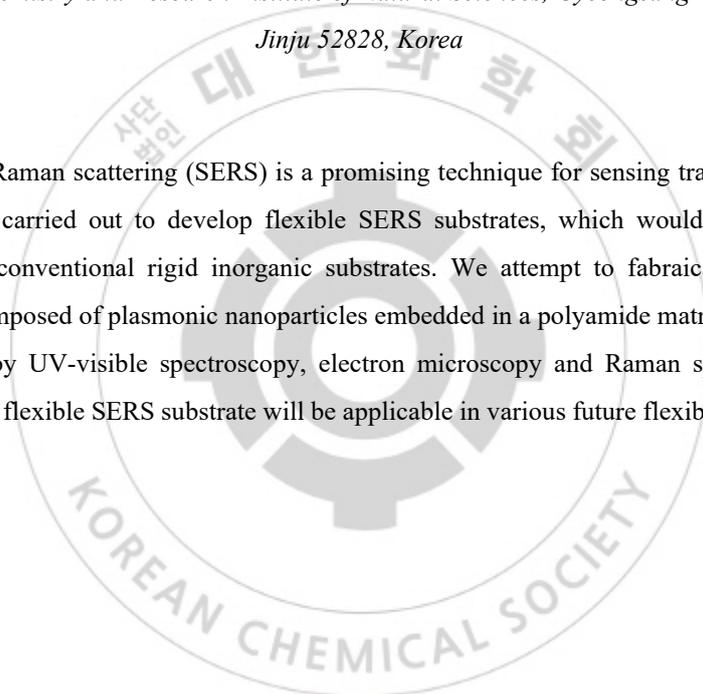
Zoom 3 FRI 16:00~17:00

Development of flexible SERS substrate with plasmonic nanoparticles

Yeram Kim, Juyeong Kim*

*Department of Chemistry and Research Institute of Natural Sciences, Gyeongsang National University,
Jinju 52828, Korea*

Surface enhanced Raman scattering (SERS) is a promising technique for sensing trace substances. Many studies have been carried out to develop flexible SERS substrates, which would have advantages in comparison with conventional rigid inorganic substrates. We attempt to fabricate a flexible SERS substrate that is composed of plasmonic nanoparticles embedded in a polyamide matrix. Such components are characterized by UV-visible spectroscopy, electron microscopy and Raman spectroscopy. Further development of the flexible SERS substrate will be applicable in various future flexible electronic devices.



Poster Presentation : **INOR.P-120**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Enhanced UV Protection with Dual-Mode Mesoporous Silica Particles Based on MCM-48

Tai yong Lee, Suk Joong Lee*

Department of Chemistry, Korea University, Korea

With acceleration of ozone depletion, UV sun-protection from daylight has become a significant well-being hazard. Although widely used sun protectants, such as avobenzone, give sensible insurance, they have often encountered restrictions such as low UV-protection efficiency, stability and bio-compatibility. Here, we have synthesized new type of nano composites based on mesoporous silicas, MCM-48, to overcome upper mentioned problems. The average size of the particles maintained ~350 nm, because this generates an ideal environment to reflect and scatter most of UV-A. In addition, avobenzone was absorbed in the MCM-48 to provide further absorption of UV-A and to enhance its stability. Note that this is the first report of the introduction of various types of phenyl (L1) and biphenyl (L2) organosilica with an extended pi orbital, which were coated by outward of MCM-48s to boost the UV absorption. Hence, the acquired outcomes reveal promising candidates of MCM-48 based composites with respect to their potential for UV protecting applications. Additionally, in-vivo investigations have been performed to show the predominant UV protecting capacity of MCM-48 based composites in examinations with a situation without any UV filters.

Poster Presentation : **INOR.P-121**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Detoxification of Chemical Warfare Agent Simulant with UV-C radiations in Liquid Phase.

Etae Choi, Hyemin Choi, Suk Joong Lee*

Department of Chemistry, Korea University, Korea

Detoxification of chemical warfare agents (CWAs) is an important part of protecting from chemical terrorism. One of the recently developed methods is the utilization of ultra violet (UV) radiations without any photo catalysts. UV is known to have enough energy to break-down or trigger the decomposition of CWAs. In particular, UV-C (100~280 nm) are good candidates because of their high energy. However, instantaneous decomposition still remains challenging when the photo-catalysts such as TiO₂ and ZnO are applied. Herein, we report a strategy for decontamination of a CWA simulant including 2-CEES (2-chloroethyl ethyl sulfide) under UV-C (277 nm) irradiation in liquid phase. 2-CEES is a simulant of mustard gas. Furthermore, we also examined a solvent effect on the decomposition such as dichloromethane (MC), acetone and acetonitrile. Interestingly, 2-CEES underwent to a non-toxic material, CEESO, with 99% conversion within 8 minutes when acetonitrile was used. Such an oxidation rate was significantly higher compared to those of the corresponding photo-decomposition researches reported so far. We also demonstrated the use of oxygen in mechanisms through the singlet oxygen scavenger experiment.

Poster Presentation : **INOR.P-122**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Photocatalytic degradation of 2-chloroethyl ethyl sulfide (2-CEES) with porphyrin-based polymer of intrinsic microporosity (PIM)

Hyemin Choi, Etae Choi, Suk Joong Lee*

Department of Chemistry, Korea University, Korea

Due to their lethality to human, the detoxification of chemical warfare agent (CWA), including Tabun (GA), Sarin (GB), Soman (GD) and VX, has been considered a major problem for decades. In particular, the mustard gas, known as blistering agent, is one of the most fatal CWAs and causes dramatic decrease in combat power. Until recently, the numerous studies have been focused on photocatalytic oxidation as one of most widely studied methods for decomposing simulant of mustard gas. For example, heterogeneous catalysts such as TiO₂, have been widely used for the degradation of CWAs. However, due to the high oxygen demand and long reaction time, more efficient system development is still required. In this presentation, the 2-CEES, which is a simulant for the mustard gas, decomposition study using porphyrin-based PIM will be demonstrated. Due to their porosity, the porphyrin-based PIM showed a quick decomposition of 2-CEES under air with 425 nm LED exposure.

Poster Presentation : **INOR.P-123**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Metal Oxide@Mesoporous Silica Composites as Catalyst for Detoxification of Chemical Warfare Agent(CWA) Simulant

Ye Ji Kim, Suk Joong Lee*

Department of Chemistry, Korea University, Korea

Materials that can destruct chemical warfare agents (CWAs) such as VX, sarin (GB), sulfur mustard (H, HT, HD), and tabun (GA) are studied for several decades. Especially, metal-organic frameworks (MOFs) have been often investigated as catalysts for CWA decomposition. However, MOFs have the drawback of relatively low stability for practical usage. In this regard, we have employed metal oxide embedded mesoporous silica (MPS) materials. Due to their structural uniqueness, metal oxide (MO) nanoparticles which have a large ratio of surface area/unit volume were attractive as the catalyst. Furthermore, these particles were non-toxic and stable. Therefore, we can prevent the agglomeration of MO nanoparticles that hinders catalytic activity by incorporating metal oxide nanoparticles into the well-ordered pores of mesoporous silica. Additionally, these composites easily separated from the reaction media. Here, we like to present the preparation of MO@MPS materials and demonstrate the decomposition of DMNP which is a sarin simulant.

Poster Presentation : **INOR.P-124**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Fabrication of patterned molybdenum via nanoimprinting method using a soft stamp, polydimethylsiloxane

Hyengjin Kim, Minji Ko¹, Selim Yun², Young rag Do^{3,*}

applied chemistry, Kookmin University, Korea

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²*Kookmin University, Korea*

³*Department of Bionano Chemistry, Kookmin University, Korea*

Today, various nano-scale products are produced through large-scale nano-patterns. There are many ways to pattern a large area. One appropriate patterning method for large area is nano-imprinting. To realize patterned molybdenum (Mo) structures, we selected the reverse nanoimprinting method, in which an imprinting resin, spin-on-glass (SOG), is spin coated on a soft stamp of polydimethylsiloxane (PDMS). The realized patterned Mo structure has a diameter of 550 nm and height of 650 nm. This structure improves the efficiency of Cu-In-Ga-Se (CIGS) solar cells by increasing the surface area. It is expected that CIGS solar cells using patterned Mo electrodes will increase surface area by separating excitons and reducing the distance between the p-n junction and the electrode.

Poster Presentation : **INOR.P-125**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Single-atom oxygen reduction reaction electrocatalysts of Fe, Si, and N co-doped carbon with 3D interconnected mesoporosity

Min seok Kang, Won Cheol Yoo*

Department of Chemical and Molecular Engineering, Hanyang University (ERICA), Korea

The development of non Pt-based catalysts (non-PBCs) that show excellent oxygen reduction reaction (ORR) activity for high-performance Zn-air battery (ZAB) and anion exchange membrane fuel cell (AEMFC) is highly necessitated. Here, the unprecedented single-atom ORR activity of Fe, Si, and N co-doped carbon (FeSiNC) supported on 3D interconnected mesoporous carbons (25 and 50 nm) derived from silica templates is reported. Si moieties connected to a carbon surface were involved in the formation of an atomically distributed $\text{FeSi}_x\text{N}_{4-x}$ site through substitution of Si at the N position in the Fe-N₄ site, which is the ORR active site of the conventional FeNC. FeSiNC with its larger mesopore (50 nm) exhibits outstanding ORR activity comparable to the most efficient non-Pt-based catalysts and enhanced single-cell performances due to its enhanced mass-transport property. According to theoretical calculations, the ORR activity is originated from not only $\text{FeSi}_x\text{N}_{4-x}$ sites located at the basal plane and inter-edge sites, but also C sites adjacent to the Si dopant in both edge and basal regions. Therefore, this study provides a facile strategy toward the rational design of inexpensive and highly active ORR catalysts applicable to single-cell devices.

Poster Presentation : **INOR.P-126**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Two novel pyridinium manganese compounds with distinct PL emissions

Myung-Ho Choi, Kang Min Ok*

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Two novel photoluminescence materials, 4A-Mn and 3A-Mn have been prepared through slow evaporation methods by using MnBr_2 , HBr and two different pyridine derivatives as reagents. 4A-Mn and 3A-Mn crystallized in the monoclinic space group, $C2/c$, and tetragonal space group, $I4_1md$, respectively. The two molecular compounds show different photoluminescence spectra attributable to the different structural environments. 4A-Mn with the typical tetrahedral unit shows a green emission, whereas 3A-Mn with the distorted trigonal bipyramidal unit exhibits a red emission. The different shapes of rigid ligands might make dissimilar H-bonding with polyhedra of Mn, which results in different photoluminescence.

Poster Presentation : **INOR.P-127**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

The Influence of Biomolecules on the Activity of Matrix Metalloproteinases

Choi Jae Yoon, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

Matrix metalloproteinases (MMPs) are known as many pathological indicators for multiple disease such as Alzheimer's diseases (AD), tumor, and glioblastoma. Among MMP family, MMP-2, gelatinase A, has been observed in AD patients' brain tissue with high level. Also, MMP-2 could degrade both amyloid precursor protein (APP) and amyloid- β ($A\beta$) which could be major causes of AD. Thus, MMP-2 has been proposed to be related to the pathogenesis of AD. In this study, we will examine the influence of various vitamins [i.e., retinol (vitamin A), pyridoxamine (vitamin B6), ascorbic acid (vitamin C), cholecalciferol (vitamin D3)] and metal ions [e.g., Fe(III), Cu(II), Zn(II)] on MMP-2's $A\beta$ degrading ability through biochemical and biophysical analysis (i.e., docking simulations, zymography, colorimetric assay, and mass spectrometry). Our overall investigation from the experiments, the effects of biomolecules on the activity of MMP-2 could help understand the relationships between metalloenzymes, particularly MMPs, and AD.

Poster Presentation : **INOR.P-128**

Inorganic Chemistry

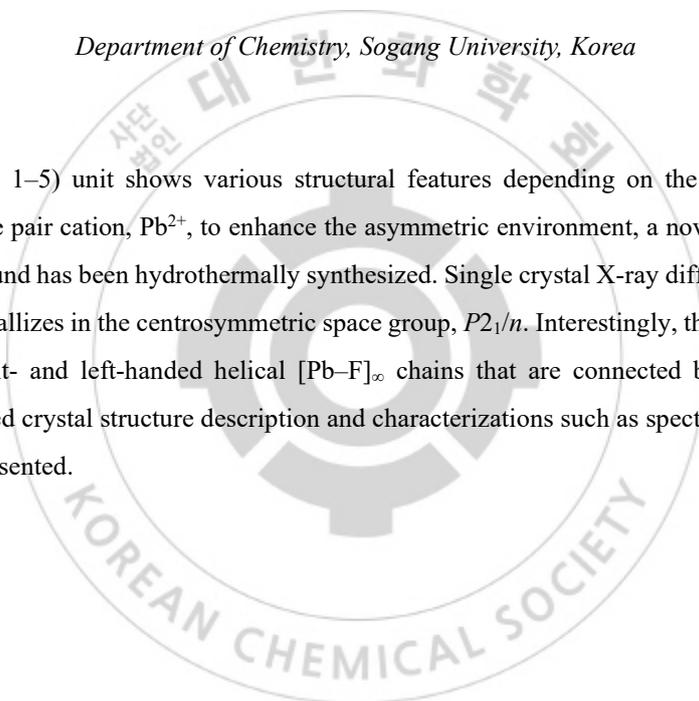
Zoom 3 FRI 16:00~17:00

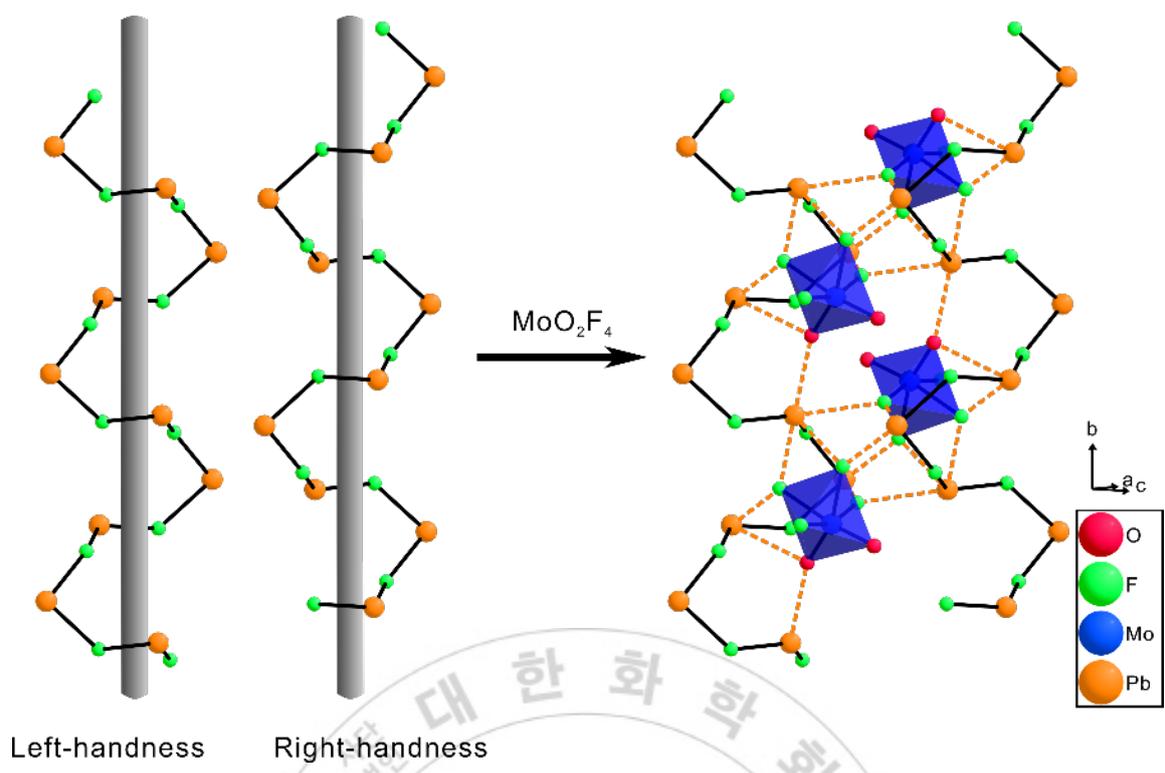
Synthesis, structure, and characterization of a new lead molybdenum oxyfluoride

Hongil Jo, Kang Min Ok*

Department of Chemistry, Sogang University, Korea

The $\text{MoO}_x\text{F}_{6-x}$ ($x = 1-5$) unit shows various structural features depending on the counter cations. By introducing the lone pair cation, Pb^{2+} , to enhance the asymmetric environment, a novel lead molybdenum oxyfluoride compound has been hydrothermally synthesized. Single crystal X-ray diffraction indicates that the compound crystallizes in the centrosymmetric space group, $P2_1/n$. Interestingly, the compound consists of both of the right- and left-handed helical $[\text{Pb-F}]_\infty$ chains that are connected by MoO_2F_4 distorted octahedra. A detailed crystal structure description and characterizations such as spectroscopic and thermal analyses will be presented.





Poster Presentation : **INOR.P-129**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Correlation between the Matrix Metalloproteinase-9 and Biomolecules

Hang Choi, Hyuck Jin Lee*

Department of Chemistry Education, Kongju National University, Korea

Matrix metalloproteinases (MMPs) have been proposed as pathological indicators for the 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 ($A\beta$) which could form toxic aggregates causing AD. In this study, we will examine the influence of multiple natural products (e.g., vitamins, metal ions) on MMPs' $A\beta$ 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 the experiments could provide better insight into the study of the MMP-9 which could cleave $A\beta$, related to AD pathology.

Poster Presentation : **INOR.P-130**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Study on crystal structures, magnetic properties and catalytic oxidation of multinuclear iron(III) and manganese(II/III) complexes with asymmetric tetradentate ligand

Ahrim Jeong, Hyosun Lee*

Department of Chemistry, Kyungpook National University, Korea

Transitional metal complexes incorporating tetradentate ligands have received much attention in chemistry because of their significant structures and potential applications such as sensor, catalysis, magnetism, chirality and gas sorption. Recently, novel two Fe(III) dinuclear complexes and a Mn(II/III) trinuclear complex, $[(\text{Hpmaep})\text{Fe}(\text{NO}_3)]_2(\text{NO}_3)_2 \cdot 2\text{MeOH} \cdot \text{H}_2\text{O}$ (**1**), $[(\text{Hpmaep})\text{Fe}(\text{N}_3)_2]_2$ (**2**) and $[(\text{pmaep})_2\text{Mn}_3(\text{OAc})_4] \cdot 2\text{MeOH}$ (**3**), have prepared by using Fe(III)/Mn(II) salts with 3-(2-hydroxyethyl-(pyridin-2-ylmethyl)amino)propan-1-ol (H_2pmaep). In **1** and **2**, two Fe(III) ions are bridged by two O atoms of ethanol groups from mono-deprotonated Hpmaep^- ligands. Complex **3** was composed of a mixed-valence linear Mn(III)-Mn(II)-Mn(III) trimer unit. In **3**, terminal Mn(III) ions are coordinated with pmaep^{2-} and acetate anions. Each terminal Mn(III) ion is connected to a central Mn(II) via covalent bridges formed by O atoms of two acetate anions and of ethanol group from the ligand. Complexes **1** and **2** display antiferromagnetic interactions between dimeric unit through the bridging oxygen atoms. Additionally, complex **3** behaves as a weakly antiferromagnetic interaction related to major exchange interaction expected between wingtip Mn(III) and central Mn(II). Furthermore, **1** shows catalytic activities for various alcohol oxidation in good yield. **2** and **3** show catalytic activities toward diverse olefins with modest to moderate yield. In this poster, we will present the detailed preparation, crystal structures, magnetic properties and catalytic effects.

Poster Presentation : **INOR.P-131**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

A Hybrid Ru(II)/ TiO₂ Catalyst for Steadfast Photocatalytic CO₂ to CO/Formate Conversion Following Molecular Catalytic Route

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Herein, we employed a molecular Ru(II) catalyst immobilized onto the TiO₂ particulates, (4,4'-Y₂-bpy)Ru^{II}(CO)₂Cl₂ (**RuP**; Y = CH₂PO(OH)₂), as a hybrid catalyst system to secure the efficient and steady catalytic activity of molecular bipyridyl Ru(II) complex-based photocatalytic system for CO₂ reduction. From series of operando FTIR spectrochemical analysis, it was found that TiO₂-fixed molecular Ru(II) complex leads to the efficient stabilization of monomeric key intermediate, Ru-hydride (LRu^{II}(H)(CO)₂Cl), and suppresses the formation of polymeric Ru(II) complex $-(L(CO)_2Ru-Ru(CO)_2L)_n-$ which is a major deactivation product produced during photoreaction via a Ru-Ru dimeric route. The active promotion of monomeric catalytic route in hetero-binary system (IrPS + TiO₂/**RuP**) that uses TiO₂-bound Ru(II) complex as reduction catalyst led to the highly increased activity and durability of photocatalytic behavior with respect to the homogeneous catalysis of free Ru(II) catalyst (IrPS + Ru(II) catalyst), giving the maximal TON of >4816 and >2228 for CO and HCOO⁻ production respectively upon addition of 16.7 vol% TEOA for 22 h.

Poster Presentation : **INOR.P-132**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Direct etherification of alcohols by Cu(II) and Cu(I) Complexes

Eun Su Chae, Jang Hoon Cho, Hong In Lee*

Department of Chemistry, Kyungpook National University, Korea

Ethers are commonly used as solvents or building blocks in organic chemistry. Williamson ether synthesis is the most well-known method to synthesize ethers from alcohols. But the method is sensitive to reaction temperatures and requires organohalides and strong base which can generate environmentally hazardous byproducts. For this reason, a direct etherification method, in which only alcohols are used as reactants were developed. This new method utilizes alcohol dehydration catalyzed by Cu(II) and Cu(I) complexes. In this study, we have developed a new ligand EbQMA (= (NE,N'E)-2,2'-(ethane-1,2-diyl)bis(N-(quinolin-8-ylmethylene)aniline)) and air stable copper complexes, [Cu(I)(EbQMA)]ClO₄ and [Cu(II)(EbQMA)]ClO₄, to be used for the etherification. Etherification products of some alcohols were monitored by NMR and GC-MS.

Poster Presentation : **INOR.P-133**

Inorganic Chemistry

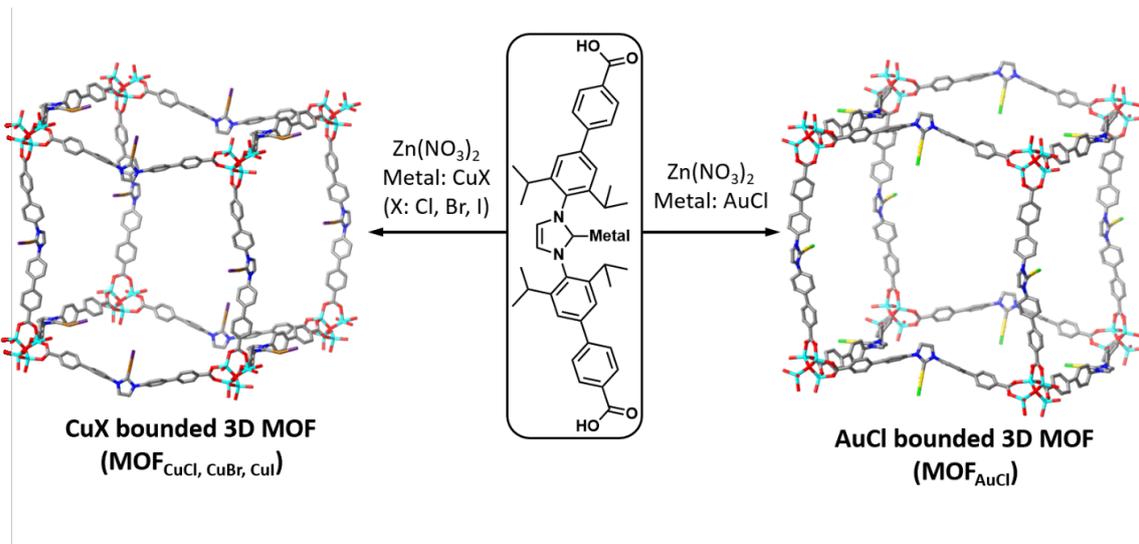
Zoom 3 FRI 16:00~17:00

De Novo Immobilization of N-Heterocyclic Carbene Metal Complexes into Metal-Organic Frameworks for Catalytic Applications

Hyunyong Kim, Eunsung Lee*

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

Metal-organic frameworks bearing N-Heterocyclic carbene transition metal complexes have been drawn attention as heterogeneous catalysts. However, most NHC metal complex embedded MOFs exhibited incomplete functionalization with desired metal complexes by in-situ deprotonation of imidazolium ligands and degradation of the framework after catalytic usage, which limits to access various transition metal NHC complexes in MOFs. Here we report a bottom-up approach to functionalize and immobilize metal complexes, including copper halides and gold chloride into MOFs in a predictable manner. The preformed NHC metal complexes, which were prepared from imidazolium ligands bearing biphenyl spacers we previously utilized for the preparation of imidazolium-based MOF, were further reacted with zinc nitrate to produce MOFs bearing the NHC metal complexes (copper halides and gold chloride). Interestingly, the resulting MOFs exhibited a similar 4-fold interpenetrated cube structure even if the types of metal complexes are different. They exhibited exceptionally high porosity despite the interpenetrated structure and high stability in organic solvents due to the multiple π - π interactions. Moreover, these MOFs exhibited high catalytic activity and size selectivity in various organic reactions including Cu-catalyzed azide-alkyne cycloaddition reaction, Cu-catalyzed multicomponent reaction, and Au-catalyzed hydroamination reaction and can be reused at least 4 times without significant loss of crystallinity and catalytic activity of the MOFs we utilized as heterogeneous catalysts. Incorporation of the various metal complexes into MOFs allows for the preparation of functional MOFs for practical applications.



Poster Presentation : **INOR.P-134**

Inorganic Chemistry

Zoom 3 FRI 16:00~17:00

Synthesis of Stability Enhanced CuInS Quantum Dots by Doping of Aluminum into ZnS Shell

Seo yeon Shin, Minji Ko, Young rag Do*

Department of Chemistry, Kookmin University, Korea

To enhance the stability of I-III-VI quantum dots (QDs), aluminum doped QDs were synthesized. These Al-doped Cu-In-S/ZnS (CIS/ZnS) quantum dots (QDs) showed an excellent photoluminescence quantum yield (PLQY) of 83%. To evaluate the effect of Al-doping, pristine CIS/ZnS QDs were also prepared. Both QDs were exposed to continuous heat and UV irradiation for 18 hours. After heating and irradiation, the pristine QDs showed efficiencies of 14% and 31% compared to the initial efficiencies. On the other hand, the Al-doped QDs showed efficiencies of 74% and 70% after the same stability test. As a consequence, Al-doped QDs can protect exposed surfaces from external factors and improve the stability.

Poster Presentation : **INOR.P-135**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Electromagnetic interference shielding (EMI-SE) of thermally conductive MXene-PAT-Poly(p-aminophenol)-polyaniline co-polymer composite.

Kanthasamy Raagulan, Younghee Park^{*}, Subin Oh^{*}, Jinsoo Kim^{1,*}, Kyu Yun Chai^{2,*}

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²*Department of Chemistry, Wonkwang University, Korea*

MXene and conductive polymers are excellent materials for EMI-SE application. The spray coating technique was utilized for the composite preparation. Different strategy has been made to develop the exfoliated MXene. The MXene-PAT-Poly(p-aminophenol)-polyaniline co-polymer (MXPATPA) composite displayed good electric conductivity (EC), heat capacity, thermal diffusivity, thermal conductivity, and thermal effusivity of 7.813 S.cm⁻¹, 2.247 J.(g.K)⁻¹, 0.282 mm².s⁻¹, 0.687 W. (m.K)⁻¹, and 1.330 W.s^{1/2}.m⁻².K⁻¹, respectively. The MXPATPA blocked 99.99% of incoming radiation and reduced form of MXene (r-Ti₃C₂T_x) enhanced the EMI-SE by 7.26%. The composites own outstanding thermal and EMI SE properties, therefore, can be applied in the application areas, such as military utensils, electronic devices, mobile phones, heat-emitting automobiles and radars.

Poster Presentation : **INOR.P-136**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

The effects of *p*-type doping for the $\text{Ca}_{2-x}\text{Na}_x\text{CdSb}_{2-y}\text{Ge}_y$ system

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The Zintl phase is one of the most promising thermoelectric materials. The Ca_2CdSb_2 structure is one of the many types of Zintl phase compounds, isostructural to the Yb_2CdSb_2 structure. Our objective is to introduce *p*-type dopants to both cationic and anionic sites to maximize carrier concentration and increase *ZT*. The Ca_2CdSb_2 structure crystallizes in the *Pnma* space group. It is composed of tetrahedral units with Cd atoms in the middle and Sb atoms on each corner, and those tetrahedral units share corners. Ca atoms exist between the tetrahedral chains. Na was chosen as the cationic *p*-dopant, whereas Ge was chosen as the anionic *p*-dopant. All compounds were synthesized via Pb molten metal flux, and characterized by both powder and single-crystal X-ray diffractions. Nicely grown bar-shaped crystals were obtained from the synthesis. The SXRD refinement showed that the Ge atoms preferred the Sb1 site and Na atoms preferred the Ca2 site. Interestingly, when the Ge concentration was above a certain level, the product was identified as the $\text{Ca}_{11}\text{Sb}_{10}$ phase. However, higher amounts of *p*-dopants did not cause any phase transition. This is due to the similar ratio of Ca and Sb between the two structures and the $\text{Ca}_{11}\text{Sb}_{10}$ phase preferring to have less electrons in its anionic framework. A series of DFT calculations using the TB-LMTO-ASA method were performed for two hypothetical structure models, $\text{Ca}_{1.5}\text{Na}_{0.5}\text{CdSb}_{1.5}\text{Ge}_{0.5}$ and Ca_2CdSb_2 for comparison. Due to being unable to measure thermoelectric properties without obtaining a single-phase product, we have devised a filtration method in addition of centrifugation to remove the flux metal. This way, after the centrifugation, the remaining lead can be slowly filtered through the quartz wool.

Poster Presentation : **INOR.P-137**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Formations of a Heterochiral Cyclic Dimer Complex and Block Homochiral Poly-pseudo-rotaxanes of *rac*-A1/A2-Difunctionalized Pillar[5]arene

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We report the first examples of coordination-directed self-assembly of pillararene-based poly-pseudo-rotaxane exhibiting chiral self-sorting behaviors. The combination of a racemic A1/A2 thiopyridyl pillar[5]arene (*rac*-L) and mercury(II) chloride afforded a heterochiral cyclic dimer complex $[\text{Hg}_2(pR\text{-L})(pS\text{-L})\text{Cl}_4] \cdot 2\text{CH}_2\text{Cl}_2$ (**1**) in which two mercury(II) atoms and one (*pR*-L)/(*pS*-L) pair make a [2:2] metallacycle via “*social*” self-sorting. Same reaction in the presence of dinitrile guest **C8**, $[\text{CN}(\text{CH}_2)_8\text{CN}]$, yielded a 1D poly-pseudo-rotaxane $\{[\text{Hg}(\text{C8}@pR\text{-L})\text{Cl}_2][\text{Hg}(\text{C8}@pS\text{-L})\text{Cl}_2] \cdot 3\text{CH}_2\text{Cl}_2\}_n$ (**2**). In **2**, *pR*-L and *pS*-L generate two separated zigzag and linear homochiral poly-pseudo-rotaxanes in a crystal, respectively, via “*narcissistic*” self-sorting. A formation pathway involving both products is proposed. Both products are new members of the pillararene family and the results could serve a better understanding of the self-sorting in nature.

Poster Presentation : **INOR.P-138**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Surface passivation of multi-shelled InP/ZnSeS/ZnS nanocrystals through simple complexing with hafnium butoxide

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³*Department of Bionano Chemistry, Kookmin University, Korea*

InP nanocrystals are promising materials for next generation display technologies. However, significant challenges remain to meet industrial demands. One major challenge is enhancing the material stability. We introduce a simple and effective strategy for surface passivation with hafnium butoxide. We first synthesized highly efficient green InP/ZnSeS/ZnS nanocrystals using a hot-injection method with a multiple injection approach. Then, surfaces were in-situ-treated with Hf(OtBu)₄. The Hf(OtBu)₄-InP/ZnSeS/ZnS nanocrystals showed photoluminescence quantum yield (PLQY) of 0.83 with a peak wavelength of 526 nm. However pristine nanocrystals showed photoluminescence quantum yield (PLQY) of 0.78 with a peak wavelength of 525 nm. Stability experiments were compared using Hf(OtBu)₄ treated InP/ZnSeS/ZnS nanocrystal solutions and pristine nanocrystal solutions under UV and thermal exposures. It was revealed that Hf(OtBu)₄ treatment is effective at enhancing the nanocrystal stability.

Poster Presentation : **INOR.P-139**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Correlation between rod length and charge transfer kinetics on metal-tipped nanorods for efficient photocatalytic hydrogen evolution

Bumjin Park, Hyunjoon Song*

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

Semiconductor-metal hybrid nanostructures have been regarded as attractive model catalysts for understanding photocatalytic hydrogen evolution because the efficiency can be varied on purpose by tailoring each part. Herein, we firstly designed the Pt tipped nanorod system to focus on the difference in reactivity according to the distance of electron acceptors. By detailed transient absorption spectroscopic study and kinetic modeling, we presented that the quantum efficiency of hydrogen generation can be expressed in terms consisting of long and short time components. As the length of the nanorod increases, the rate constants for carrier transport decrease, but the absorption cross-section increases. Therefore, the number of carriers migrating to the metal tip for the hybrid systems is optimal at 15-20 nm per tip. Our finding successfully demonstrated the exact role of the number matter of cocatalysts for ideal design of photocatalyst.

Poster Presentation : **INOR.P-140**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Synthesis of nickel doped Co-catalysts derived from MOF for the Oxygen reduction and evolution reactions in alkaline medium

Gyungse Park^{*}, Sheraz Ahmed¹

Department of Chemistry, Kunsan National University, Korea

¹Chemistry, Kunsan National University, Korea

Co-MOF was synthesized by using H₂SDA and Co (ClO₄)₂·6H₂O and then direct calcination of Co-MOF at various temperatures resulted in the preparation of Co-catalysts for the OER (oxygen evolution reaction) and ORR (oxygen reduction reaction) in zinc-air batteries. The formation of metallic Co species was investigated by the X-ray diffraction (XRD). The resulting Co-catalysts are highly porous with a high specific surface area of 165.85 m²/g at 800°C. After calcination, Ni deposition was performed, to produce Ni/H800 on which Ni-atoms are deposited on the surface of Co-catalysts. The surface area reduces to 99.60 m²/g at 800°C and the structure is distorted due to deposition. Furthermore, the Ni/H800 catalyst exhibited superior electrochemical performance as a cathode material for the zinc-air batteries. The cyclic test for charging and discharging was performed for 350 h revealing a potential catalyst, having splendid stability for the OER and ORR in the Zn-air batteries.

Poster Presentation : **INOR.P-141**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Structural interconversion of palladium(II) coordination cages by anion exchange

Haeri Lee

Department of Chemistry, Hannam University, Korea

In many different chemical processes, the control of reversible anion exchanges plays a key role in increasing the reaction rate and efficiency. Therefore structural interconversion for driving the multi-functional properties of molecular systems working on condition-based control is a hot topic for molecular engineers and scientists. However, anion exchange/recognition is very sensitive to diverse factors such as the charge of anion, size, geometry, media, temperature, pH, and inner space cavity. Thus, it is a key point to construct well-defined and flexible host coordination cages that are both appropriately sized and located. Herein, we present an unprecedented novel approach to the control of the adsorption of anions showing significant structural conversion as systematically.

Poster Presentation : **INOR.P-142**

Inorganic Chemistry

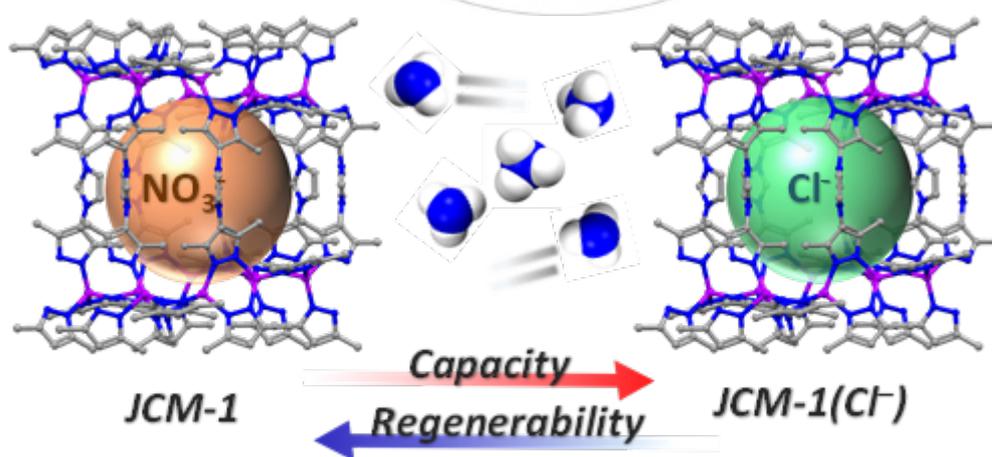
Zoom 4 FRI 15:00~16:00

Reversible Ammonia Uptake at Room Temperature in a Robust and Tunable Metal-Organic Framework

Younggyu Seo, Eunsung Lee*

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

Ammonia is the second most-produced chemical in the world, but the effective removal of ammonia from atmosphere is also important because of its high toxicity and corrosiveness. Although metal-organic frameworks (MOFs) have emerged as a strong candidate for NH₃ adsorbents, most of MOFs suffer from a lack of stability and high regeneration temperatures. Here, we report the recyclable and tunable ammonia adsorption using a robust imidazolium-based MOF (JCM-1). JCM-1 shows reversible NH₃ uptake which can be easily regenerated at room temperature without any structural deformation. Furthermore, we demonstrated the control of NH₃ adsorption affinity and uptake capacity of JCM-1 by simple ion substitution in a post-synthetic manner. To understand the anion effect on NH₃ sorption in JCM-1, interaction energies of the frameworks toward NH₃ before and after ion substitution were simulated by density functional theory (DFT) calculations.



Poster Presentation : **INOR.P-143**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Highly electrical conductive WS₂ film growth by sulfurization of tungsten film using diethyl sulfide

Yoobeen Lee, Jin Seok Lee*

Department of Chemistry, Hanyang University, Korea

The reduction of intrinsic defects, including vacancies and grain boundaries, remains one of the greatest challenges to produce high-performance transition metal dichalcogenides (TMDCs) electronic systems. A deeper comprehension of the underlying reaction mechanisms is also needed. In this work, we present a new sulfurization process of tungsten (W) film using a sulfur (S)-containing organic precursor for the growth of WS₂ films on SiO₂/Si substrates. The W film was deposited with precise layer thickness control by atomic layer deposition and uniformly sulfurized using diethyl sulfide (DES) as S precursor. Comprehensive optical and chemical analyses revealed that by using DES as S precursor, the S atoms were uniformly supplied, and sulfurization occurred accurately and delicately. Moreover, the WS₂ film synthesized using DES showed outstanding electrical conductivity (~37 mS cm⁻¹), which was almost 17 times higher than that of the WS₂ film synthesized using S powder. Based on the results of optical, electrical, and chemical analyses, we proposed and validated a hypothesis to explain the sulfurization mechanism. The fabricated TMDC materials using the method presented in this work show great potential for industrial application due to their highly uniform surface and improved electrical conductivity.

Poster Presentation : **INOR.P-144**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

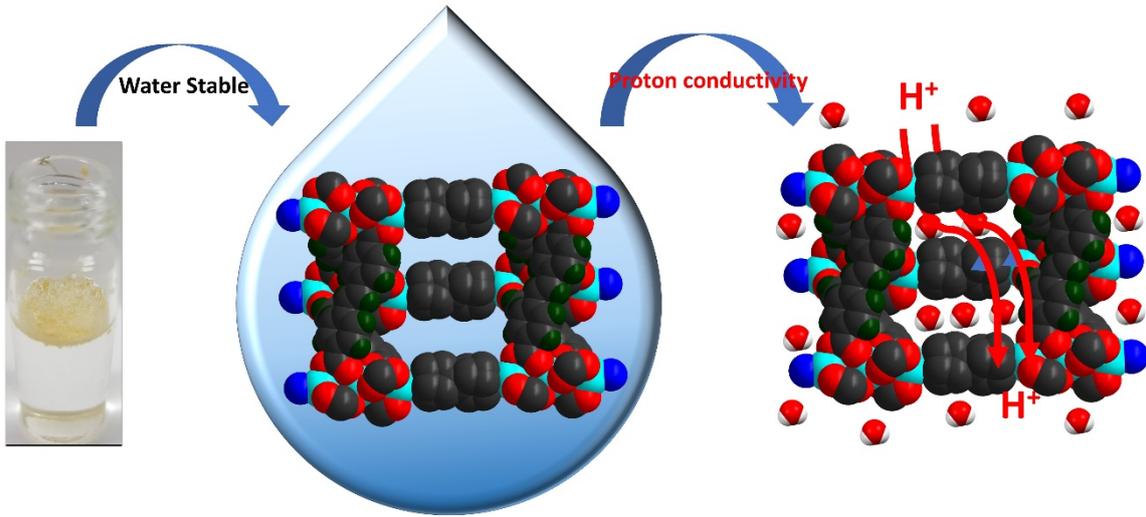
Investigation of Water Stability and Proton Conductivity of a Triply Interpenetrated Zn-based Metal-Organic Framework

Jiyun Kim, Younghu Son, Purnachandra Rao Varikuti, Gyungse Park^{1,*}, Minyoung Yoon^{*}

Department of Chemistry, Kyungpook National University, Korea

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

Among the various types of solid-state proton conductors (SSPCs), metal-organic frameworks (MOFs) have emerged as high performance and safety in the field of proton-exchange membrane fuel-cell (PEMFCs) applications. PEMFCs engender minimal pollutant emissions and environmentally benign water during energy generation. Because most of the MOFs are enduring instability in water media, there is an urgent need to develop water stable MOF-based SSPCs in the field of fuel cell applications. Herein, we present a three-dimensional trinuclear zinc-based metal-organic framework and its water stability, which is denoted as Zn-SDC-MOF by using modified reported synthetic conditions, where stilbenedicarboxylic acid (H₂SDC) and 4,4'-bipyridine (bpy) are employed as organic linker units. The H₂SDC is a long chain ligand that is attributed to synthesize flexible coordination geometries and trinuclear Zn-MOFs possesses exceptional stability in air compared to the MOF comprising Zn₄O SBUs as reported by Allendorf and co-workers. Interestingly, the Zn-SDA MOF shows high stability in water (at least 4 weeks) and basic aqueous solution (at pH 10). By the motivation of the air stable trinuclear Zn-SDC MOF, we investigated the exceptional water stability of this MOF compound as confirmed by PXRD analysis. Moreover, the MOF has shown modest proton conductivity ($0.8 \times 10^{-3} \text{ S cm}^{-1}$) at 95% relative humidity (RH) and 298 K with the activation energy of 0.36 eV. Therefore, the triply interpenetrated MOF with water stability and better proton conductive performance can draw significant attention for the application of PEMFCs.



Poster Presentation : **INOR.P-145**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Morphology Transformation of Ag⁺-Coordinated Supramolecular Polymer through terpyridine-based ligand

Chenxing Li, Jong Hwa Jung*

Department of Chemistry, Gyeongsang National University, Korea

We present a unique dynamic morphology of Ag⁺-coordinated supramolecular nanostructure at two different concentrations of AgNO₃. In the presence of AgNO₃(0.5 equiv.), the chiral terpyridine-based ligand (**1**), generated a fiber structure, which led to the generation of a CD signal with right-handed (P-type) helicity. In the presence of AgNO₃ (1 equiv.), we observed a morphology transformation of Ag⁺-coordinated supramolecular nanostructure. A particle structure (nanostructure I) was preferentially generated based on the **1**₂Ag complex (**1**:Ag⁺ = 2:1) as a metastable product. This nanostructure I was then transformed into nanostructure II after aging for several hours, which was composed of the **1**Ag complex (**1**:Ag⁺ = 1:1) as the thermodynamically stable product. This nanostructure exhibited a ring-like structure with a uniform diameter, which led to the generation of a CD signal with left-handed (M-type) helicity.

Poster Presentation : **INOR.P-146**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Synthesis and Metallation of Bidentate Cyclic (Alkyl)(Amino)Carbenes (cAACs)

Jang Minjae, Dae Young Bae¹, Hayoung Song¹, Eunsung Lee^{1,*}

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

Cyclic (alkyl)(amino)carbenes (cAACs) have attracted remarkable attention because of their more outstanding σ -donating and π -accepting ability than N-heterocyclic carbenes (NHCs). By replacing one nitrogen atom with one carbon atom, these carbenes become more nucleophilic as well as electrophilic. Through this, cAACs could successfully stabilize low valent metal complexes or organic radicals. Unlike NHCs, recently synthesis of bidentate cAACs was reported by Bertrand group due to synthetic difficulties. Although this distinguished work, the application of these bidentate cAACs remains rare. Herein, we report the new metal complex bearing bidentate cyclic alkyl amino carbene. The metal complex was characterized by NMR spectroscopy and single-crystal X-ray diffraction analysis. Reactivity of this metal complex will be presented.

Poster Presentation : **INOR.P-147**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

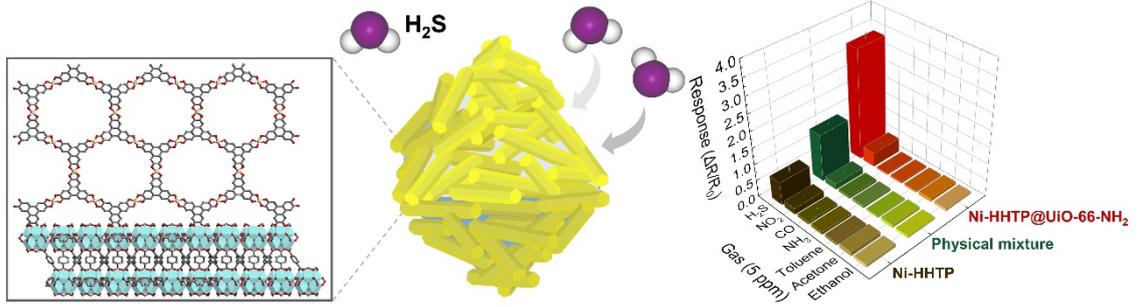
Multi-Dimensional Integration of Conductive 2D MOF on Porous 3D MOF Structures: Superior Room Temperature Chemiresistor

Sujee Cho, Hoi Ri Moon*, Jaehwa Lee

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

Chemical sensing of toxic gases is necessary for use in applications such as air pollution monitoring, food quality management, and disease diagnosis. Although some viable sensors for toxic gases have been reported, research to develop ideal sensing devices is still on the rise with grand challenges unfulfilled: ppb-level sensitivity, accurate target gas detection, and long-term stability. Amongst various candidate materials, metal-organic frameworks (MOFs) have opened up promising vistas as chemiresistive sensors due to their high structural and functional tunability. In this study, we report for the first time the combination of dimensionally and functionally different two MOFs in the form of core-shell structure. A two-dimensional (2D) conductive MOF (Ni-HHTP, HHTP = 2,3,6,7,10,11-hexahydroxytriphenylene) is synthesized on a three-dimensional (3D) porous MOF (UiO-66-NH₂) via seed-mediated growth on the ligand-functionalized surface, resulting in the synthesis of the well-integrated 2D-MOF@3D-MOF composite that possesses high conductivity and large surface area simultaneously. This hierarchically assembled heterostructure exhibits greatly enhanced sensing performances toward toxic H₂S gas with the lowest limit of detection (1.4 ppb) as well as superior sensitivity ($\Delta R/R_0 = 3.36$) and selectivity at room temperature in air. This effective chemiresistive sensor is achieved by unique redox properties derived from free radicals at the interface as well as a synergistic effect of high conductivity and large surface area attributed to the heterostructure.

Superior RT Chemiresistor, Multidimensional Composite Ni-HHTP@UiO-66-NH₂



Poster Presentation : **INOR.P-148**

Inorganic Chemistry

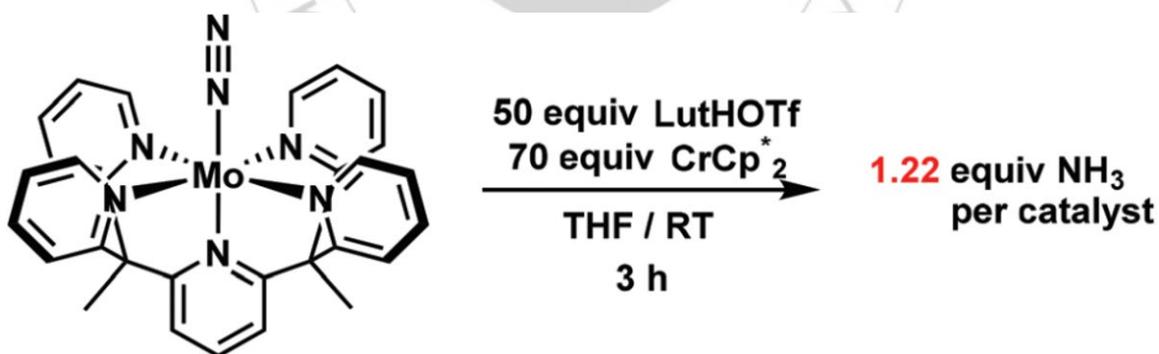
Zoom 4 FRI 15:00~16:00

Dinitrogen Activation by Penta-pyridyl Molybdenum Complex

Jeongmin Cha, Hayoung Song, Eunsung Lee*

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

A new dinitrogen (N₂) molybdenum(0) complex supported exclusively by pyridine ligands was synthesized. The X-ray crystal structure of the complex elucidated the activated nature of the N₂ ligand, consistent with a low N–N IR stretching frequency. Natural bond orbital (NBO) analyses on this system confirmed a strong π -backdonation arising from the large p orbital character in molybdenum lone pairs. 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-149**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

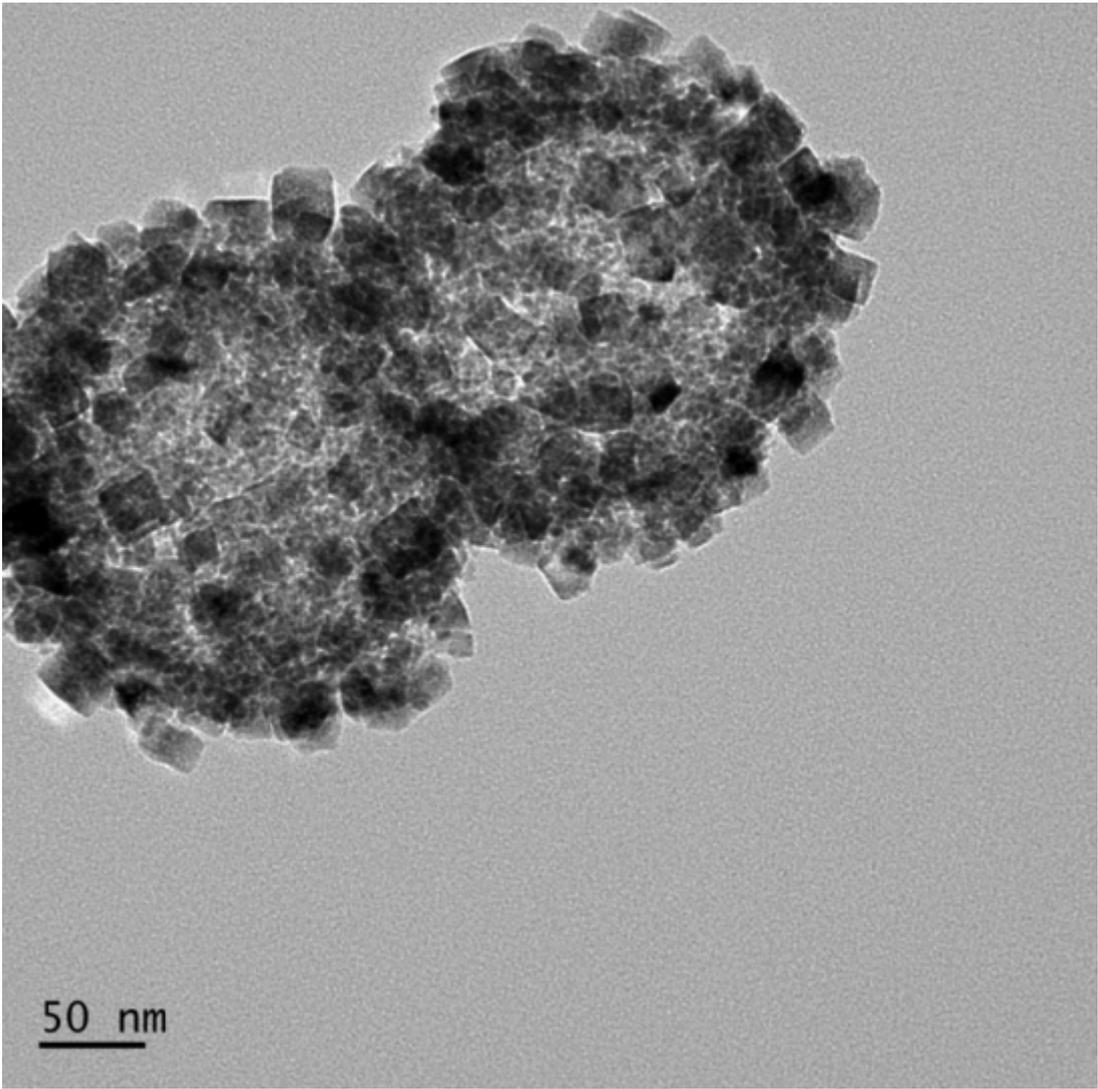
Full-wavelength photoconversion of CO₂ by colloidal nanocatalysts

Byeonghoon Choi, Hyunjoon Song^{1,*}

chemistry, Korea Advanced Institute of Science and Technology, Korea

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

Generating alternative energy from the greenhouse gases is promising environmental technology. Semiconductor-mediated photocatalysis has been intensively studied due to its great potential for treating solar energy. We focused on photoreduction of CO₂ into fuels such as methane or carbon monoxide. For preventing charge recombination and improving efficiency, Z-scheme heterojunction is preferred. We synthesized ZnO@Cu₂O, hollow TiO₂@Cu₂O and g-C₃N₄@Cu₂O nanostructures. These photocatalysts exhibit high photocatalytic activities and selectivities under ultraviolet light irradiation. Furthermore, for utilizing more solar energy, we propose to expand our research area to visible light-responsive photocatalysis. We synthesized hollow TiO₂@Cu₂O@Au photocatalysts catalyzed CO₂ reduction under visible light irradiation.



Poster Presentation : **INOR.P-150**

Inorganic Chemistry

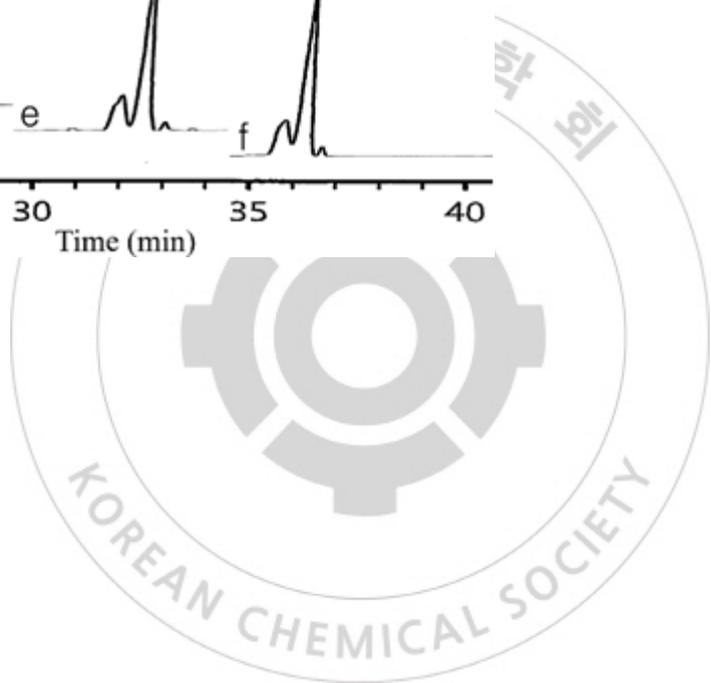
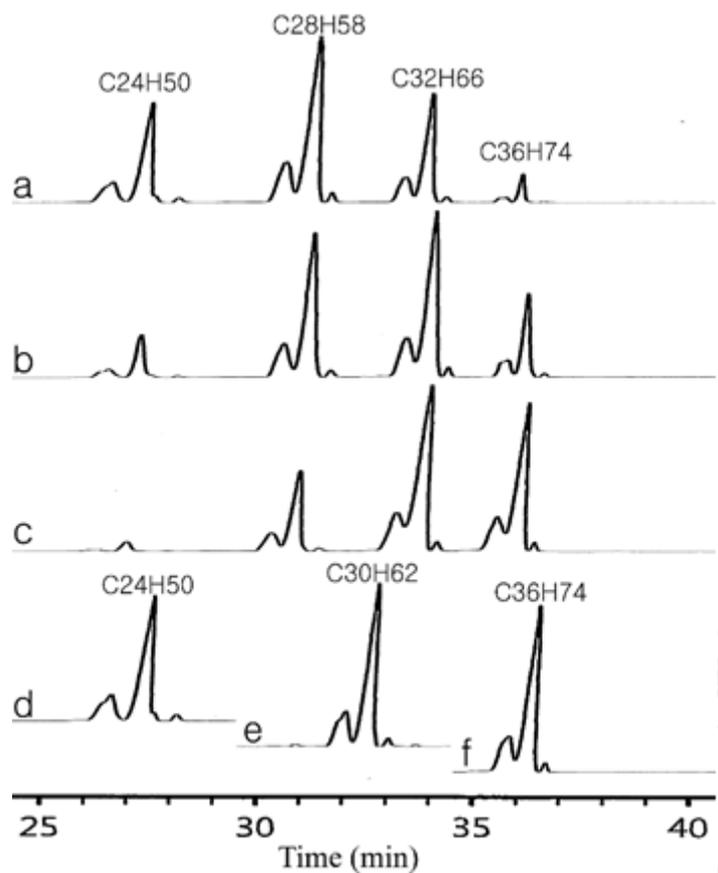
Zoom 4 FRI 15:00~16:00

Selective Trimerization of α -Olefins with Supported Chromium Catalyst for Lubricant Base Oils

Jun Won Baek, Bun Yeoul Lee*

Department of Molecular Science and Technology, Ajou University, Korea

The demand for poly(α -olefin)s (PAOs), which are high-performance group IV lubricant base oils, is progressively high. PAOs are generally produced via the cationic oligomerization of 1-decene, wherein skeleton rearrangement unavoidably occurs in the products. Therefore, a transition-metal-based catalytic process avoiding rearrangement would be a valuable alternative for cationic oligomerization. In particular, transition-metal-catalyzed selective trimerization of α -olefins has the potential for success. In here, (*N,N,N'*-tridodecyltriazacyclohexane)CrCl₃ complex was reacted with MAO-silica (MAO, methylaluminoxane) for the preparation of a supported catalyst, which exhibited superior performance in selective α -olefin trimerization compared to that of the corresponding homogeneous catalyst, enabling the preparation of α -olefin trimers at ~200 g scale. Following hydrogenation, the prepared 1-decene trimer (C₃₀H₆₂) exhibited better lubricant properties than those of commercial-grade PAO-4 (kinematic viscosity at 40 °C, 15.1 vs. 17.4 cSt; kinematic viscosity at 100 °C, 3.9 vs. 3.9 cSt; viscosity index, 161 vs. 123). Furthermore, it was indicated that 1-octene/1-dodecene mixed co-trimers (i.e., a mixture of C₂₄H₅₀, C₂₈H₅₈, C₃₂H₆₆, and C₃₆H₇₄), produced by the selective supported Cr catalyst, exhibited outstanding lubricant properties analogous to those observed for the 1-decene trimer (C₃₀H₆₂).



Poster Presentation : **INOR.P-151**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Dinuclear metallocene complex for highly efficient catalyst using silica-MAO

Sun Mi Jeong, Bun Yeoul Lee*

Department of Molecular Science and Technology, Ajou University, Korea

For application in mercantile slurry and gas-phase processes, single-site homogeneous metallocene catalysts are typically immobilized on silica surfaces to control the size and morphology of the generated polymer particles. However, the main challenge limiting the commercialisation of these catalysts is the enhancement of their productivity (measured in kg-PE/g-(supported catalyst)). Herein, we demonstrate that the output of supported catalysts can be enhanced by using dinuclear metallocene complexes instead of the conventional mononuclear analogs to prepare the supported catalysts. Thus, the productivity of the supported catalysts prepared by reacting methylaluminoxane (MAO)-treated silica (denoted as silica-MAO) with dinuclear ansa-metallocene complexes synthesized with silylene-bridged and thiophene-fused cyclopentadienyl ligands was almost twice that of the catalysts prepared with the mononuclear analogs. The enhanced output is because of the higher loading of the dinuclear complexes than that of the mononuclear analogs; the fed dinuclear complexes were entirely anchored on silica-MAO at 90–150 $\mu\text{mol-Zr/g-(silica-MAO)}$ feed, whereas only a part of the fed mononuclear metallocene complexes was anchored on silica-MAO even at 90 $\mu\text{mol-Zr/g-(silica-MAO)}$ feed. In addition, the supported catalysts prepared with the dinuclear complexes suppressed the formation of large polymer particles.

Poster Presentation : **INOR.P-152**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Synthesis of New Stable Organic Radicals

Junbeom Park, Eunsung Lee*

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

Organic radicals have attracted great attention due to their unique reactivity and properties. Typically, organic radicals present low stability and solubility, it often became a barrier to deep understanding of their properties and further applications. Especially, the stability toward biological redox reagents and the solubility toward water are essential for physiological application. Recently, our group introduced the 1,2-dicarbonyl radicals supported by two *N*-heterocyclic carbene units which exhibit exceptional physiological and chemical stability. Herein, we report the new 1,2-dicarbonyl radicals supported by a bidentate *N*-heterocyclic carbene unit. The reaction between bidentate *N*-heterocyclic carbenes and oxalyl chloride affords corresponding 1,2-dicarbonyl radicals which present better solubility toward water and high stability. The detailed synthesis and full characterization of the radicals including EPR spectroscopy will be presented.

Poster Presentation : **INOR.P-153**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Controlling the degree of doping on Ru-based nanocatalysts as active electrocatalysts toward the oxygen evolution reaction

Songa Choi, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Since the concerns about fossil fuel consumption and related environmental issues are growing, the production of sustainable and renewable green energies has been regarded as a critical strategy for alternating the conventional carbon-based energies. Water electrolysis is a promising technique for producing hydrogen energy. However, the hurdle in improving water electrolysis is primarily caused by the sluggish reaction kinetics of the oxygen evolution reaction (OER). Recently, in the case of related Ru oxides, the presence of small amount of leaching-resistant heteroatom in the oxide matrix was conducive to the high stability of Ru oxide-based catalyst. However, the strategy methods of heteroatom doping in the oxide matrix have not deeply been developed as far. Thus, in this study, we designed that the Pt doped RuO₂ nanocatalysts induced by oxophilic transition metals might be essential toward the OER under acidic conditions. With the introduction of transition metals, heteroatom in the sublayer of the surface can be easily moved into the RuO₂ shell during the thermal oxidation process. The presence of heteroatoms in the Ru oxide matrix appears to be beneficial on the catalyst activity and stability by mitigating the Ru dissolution.

Poster Presentation : **INOR.P-154**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

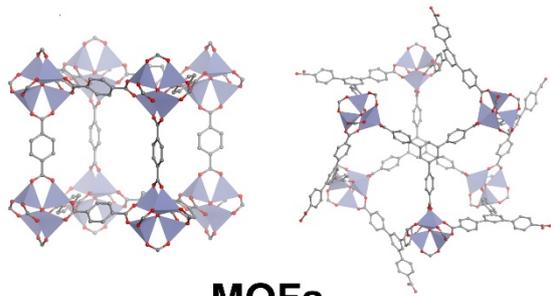
Mechanochemistry as a Reconstruction Tool of Decomposed Metal–Organic Frameworks

HongKyu Lee, Jaehwa Lee¹, Hoi Ri Moon^{1,*}

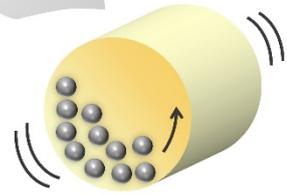
Chemistry, Ulsan National Institute of Science and Technology, Korea

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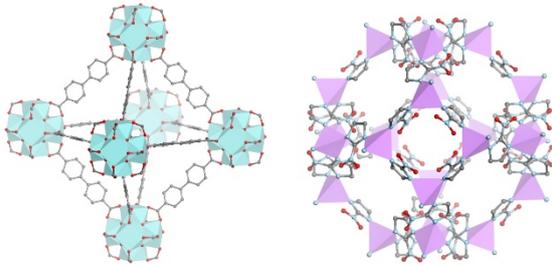
These efforts to develop synthetic strategies for more stable MOFs have significantly expanded the practical applications of MOFs. Nevertheless, these “stable MOFs” are still less stable than other industrially viable porous materials, including zeolites and activated carbons. The crystalline structures of MOFs tend to degrade under harsh conditions, including moisture and acidic/alkaline solutions, and upon repetitive operation/activation cycles. Considering the current state of development of stable MOFs, the recycling of degraded MOFs presents a meaningful approach in a different direction toward industrializing these promising materials. This should be also beneficial because deteriorated MOFs can themselves be hostile to the environment as toxic residues. Herein, we present mechanochemical strategies for the reconstruction of four selected metal–organic frameworks (MOFs) (MOF-5, MOF-177, UiO-67, and ZIF-65). To verify the effectiveness of this approach, these MOFs were intentionally decomposed in aqueous media and subsequently treated by ball milling under optimized conditions. As confirmed by X-ray diffraction analysis and N₂ sorption isotherms, regardless of the MOF degradation pathway, the original structure could be recovered by a tailored mechanochemical reaction. This approach expands the recyclability and practical applications of MOFs by enabling the regeneration of deteriorated MOFs quickly at a large scale.



Decomposition



Ball milling



Reconstruction



Poster Presentation : **INOR.P-155**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Eco-friendly heavy-metal-free perovskite for highly emissive phosphor

Hyeongjin Lee, Sang Wook Park¹, Young rag Do^{2,*}

Department of Applied Chemistry, Kookmin University, Korea

¹*Department of Chemistry, Kookmin University, Korea*

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Perovskites are promising materials for lighting applications because of their high photo luminescent quantum yields (PLQYs), narrow full-width at half maximum (FWHM) and easy synthesis. However, almost all-inorganic perovskite QDs involve heavy metals, such as Cd and Pb. These heavy metals are very harmful to human health, the eco system and the environment. For this reason, these materials are prohibited by RoHS regulations. Therefore, a lot of research has been conducted on perovskites without heavy metals. However, it has been difficult to achieve high efficiency without heavy metals such as Cd and Pb. Here, we suggest eco-friendly heavy-metal-free perovskites for highly emissive phosphors. We used Cu instead of Pb. The Photo-Luminescent Quantum Yield (PLQY) of the perovskite that we synthesized was 74%, and the peak wavelength of emission light was 448nm, and the Full Width at Half Maximum (FWHM) was 65nm. After air stability test 15days, PLQY was 95% of initial PLQY. Due to the high PLQY, narrow FWHM, suitable wavelength and easy synthesis, this material will be used in phosphor applications for lighting or displays.

Poster Presentation : **INOR.P-156**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Synthesis of Cs₃MnBr₅ through air-free baking

Sang wook Park, Hyeongjin Lee¹, Heejoon Kang², Young rag Do^{2,*}

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²*Department of Bionano Chemistry, Kookmin University, Korea*

Perovskite nanocrystals, such as cesium lead halide, are promising emissive materials in the lighting and display field. However, cesium lead halide perovskites present certain problems. Lead, used to synthesize cesium lead halide perovskite, is harmful to humans, animals, and the environment. The European Union (EU) prohibits the use of lead in electronic devices. Therefore, perovskite research based on eco-friendly materials is becoming meaningful. In papers published so far, Cs₃MnBr₅ has usually been synthesized through evaporative crystallization. In this paper, we used solid-state chemistry to synthesize Cs₃MnBr₅. First, we mixed cesium bromide (CsBr) and manganese bromide (MnBr₂). Second, we put the mixed powder in a crucible and baked it in a furnace in air-free condition. After baking and cooling, we observed that a light green powder was synthesized and green luminescence of that in UV-lamp (365nm excitation). The photoluminescence quantum yield (PLQY), emission wavelength and full width at half-maximum (FWHM) of the emissive powder were 15%, 516 nm and 41 nm.

Poster Presentation : **INOR.P-157**

Inorganic Chemistry

Zoom 4 FRI 15:00~16:00

Advanced NO₂ sensor Performance via Newly Synthesized MOF-derived Carbon Nanofibers

Miyeon Kim, Chang Yeon Lee*

Department of Energy and Chemical Engineering, Incheon National University, Korea

Metal organic frameworks (MOFs), constructed via self-assembly by inorganic secondary building units and organic ligand units, have emerged as an innovative porous material. Their enormous surface area, ordered structure, adjustable pore size and properties make it suitable for a variety of applications such as gas storage, separation, sensing, drug delivery or catalysis. In particular, MOFs-derived carbon materials are useful for catalyzing electric reactions by reducing the insulating properties of MOFs. On the other hand, the organic transistor-based gas sensor has the advantage of being light, flexible, and capable of detecting harmful gases by simply controlling the current, but has the disadvantage that the sensor characteristic is low due to a low degree of crystallinity and the electrical conductivity of the conjugated polymer to be used as an active layer. In this study, we synthesized Z67@CNF with a new method using cobalt-porphyrin. In addition, poly(3-hexylthiophene), which is a conjugated polymer, and Z67@CNF were mixed for an active layer to analyze harmful gas adsorption and charge transfer characteristics of transistors. We can found that Z67(ZIF67) synthesized on CNF exhibited high reactivity to NO₂ due to improved dispersion and electrical conductivity by CNF.

Poster Presentation : **INOR.P-158**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Synthesis of β -NiOOH on Ni nanoplates and their application towards the Oxygen Evolution Reaction

Hye Jin Lee, Sang-II Choi*

Department of Chemistry, Kyungpook National University, Korea

Recently, the development of eco-friendly energy has been accelerated with the increasing awareness for the environment. Because hydrogen is a major component of eco-friendly energy, the reactions of water electrolysis consisting of oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), have become significant. Especially, OER requires appropriate catalysts to make the reaction more efficient as it has complex mechanisms and intermediates compared to HER. Iridium and ruthenium were mainly used for OER catalysts, but both of them have limited deposit and are expensive. Therefore, relatively abundant and cheap metals have been applied, and nickel is one of the most promising candidates. Previous studies showed that β -NiOOH grown on Ni(111) facet exhibited good OER performance and well maintained its structure during reaction. Herein, we synthesized Ni nanoplates with dominant Ni(111) facet and made the β -NiOOH layers on the surface of Ni nanoplates by electrochemical oxidation. The layered β -NiOOH structure was confirmed by high resolution-transmission electron microscopy, X-ray scattering, and X-ray photoelectron spectroscopy. Layered β -NiOOH on Ni nanoplates showed enhanced OER activity and durability compared to the commercial IrO₂.

Poster Presentation : **INOR.P-159**

Inorganic Chemistry

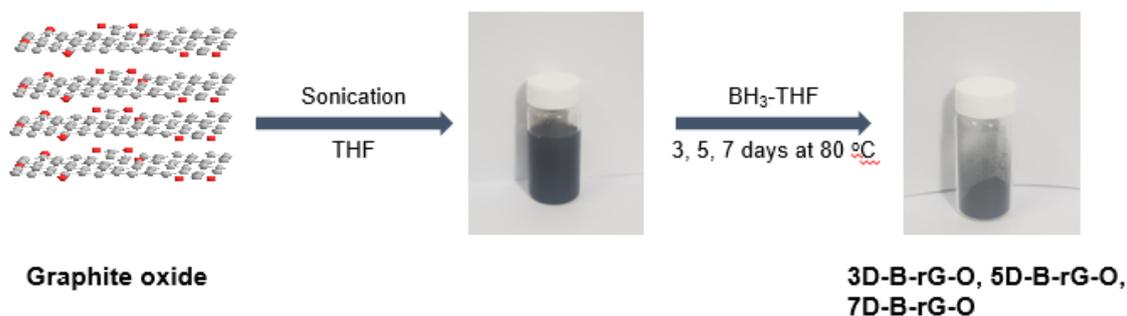
Zoom 4 FRI 16:00~17:00

Synthesis of B-doped reduced graphene oxide using wet process in tetrahydrofuran

Yunseok Shin, Sungjin Park*

Department of Chemistry, Inha University, Korea

Graphene-based materials show outstanding properties in various applications because of their electrical properties, large surface areas, and high tolerance for chemical modification and the use of wet-process is a promising way for their mass production. Heteroatom-doping is one of the common methods to improve their electrical, physical, and electrochemical properties. In this work, we introduce a new route for the synthesis B-doped graphene-based materials using low-temperature wet-process, which is the reaction between graphene oxide suspensions and a BH₃ adduct in tetrahydrofuran under reflux. Elemental mapping images show well-dispersed B atoms along the materials. Various spectroscopic characterizations confirm the reduction of the graphene oxide and incorporation of B atoms into the carbon network as high as ~2 at%. The materials showed electrocatalytic activity for oxygen reduction reactions.



Poster Presentation : **INOR.P-160**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Dopant-assisted modulation of the Ir and Ru oxidation states in oxide-based heterostructures toward oxygen evolution reaction

Ye Ji Park, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Designing an efficient and durable electrocatalyst for the sluggish oxygen evolution reaction (OER) is mandatory for clean and sustainable alternative energy sources. Herein, we reported a highly active and durable cactus-like heterostructure with an exposed heterointerface between the IrO₂ and Ru. The initial mixing of the Ir and Ru phase before the electrochemical oxidation, which is important for conjoining Ru/IrO₂ heterointerfaces, was successfully carried out by introducing dopant. This electrocatalyst exhibited high activities with a low overpotential of 198 mV at 10 mA cm⁻² and the long-term stability for over 180 h toward OER in acidic media, which surpasses those of previously reported catalysts. The results of the excellent catalytic performance for acidic OER were attributed to the synergistic effect driven by the heterostructuring robust rutile IrO₂ and highly active Ru species with a low oxidation state on the catalyst surface.

Poster Presentation : **INOR.P-161**

Inorganic Chemistry

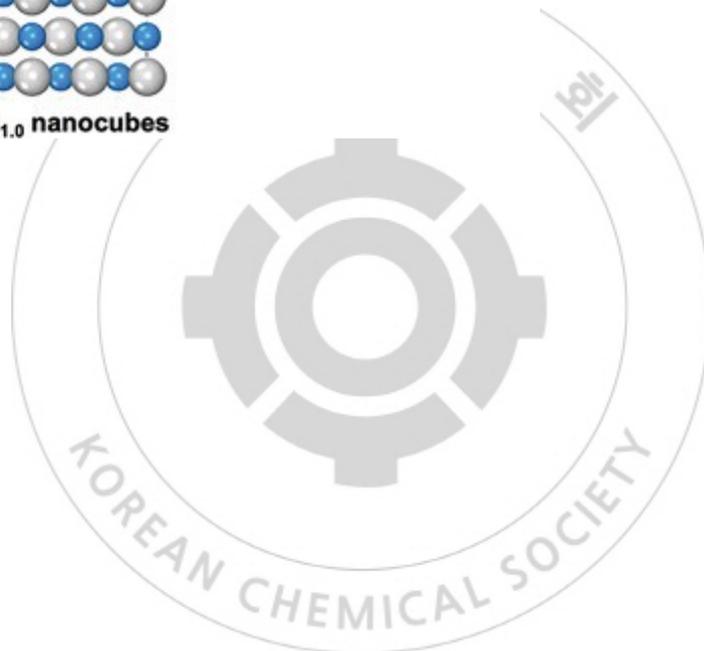
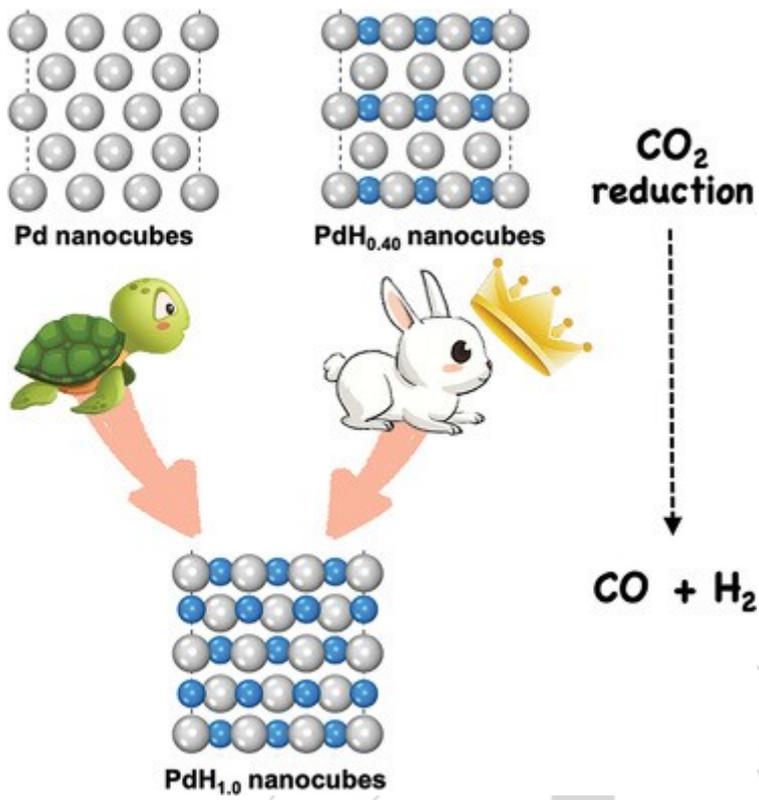
Zoom 4 FRI 16:00~17:00

Pre-hydrizing Effect on Pd Nanocubes towards the CO₂ electroreduction

Jeonghyeon Kim, Sang-II Choi*

Department of Chemistry, Kyungpook National University, Korea

The electrochemical CO₂ reduction reaction (CO₂RR) to syngas represents a promising solution to mitigate CO₂ emissions and manufacture value-added chemicals. Palladium (Pd) has been identified as a potential candidate for syngas production via CO₂RR due to its transformation to Pd hydride under CO₂RR conditions, however, the pre-hydrized effect on the catalytic properties of Pd-based electrocatalysts has not been investigated. This presentation reports the pre-hydrized PdH_{0.4} nanocubes embedded carbon black (PdH_{0.4} NCs/C) is prepared from a chemical reduction method. PdH_{0.4} NCs/C exhibited 77% and 220% enhanced CO/H₂ ratio and CO₂RR performance compared with the Pd counterpart, respectively. In-situ X-ray absorption spectroscopy reveals that higher CO/H₂ ratios and CO₂RR activity for PdH_{0.4} NCs/C were due to its less cathodic phased transformation to PdH₁. The size effects of Pd NCs were also investigated and suggesting that smaller-sized NCs show higher CO₂RR performance, because of their more abundant active sites (edge and corner sites) for CO₂RR.



Poster Presentation : **INOR.P-162**

Inorganic Chemistry

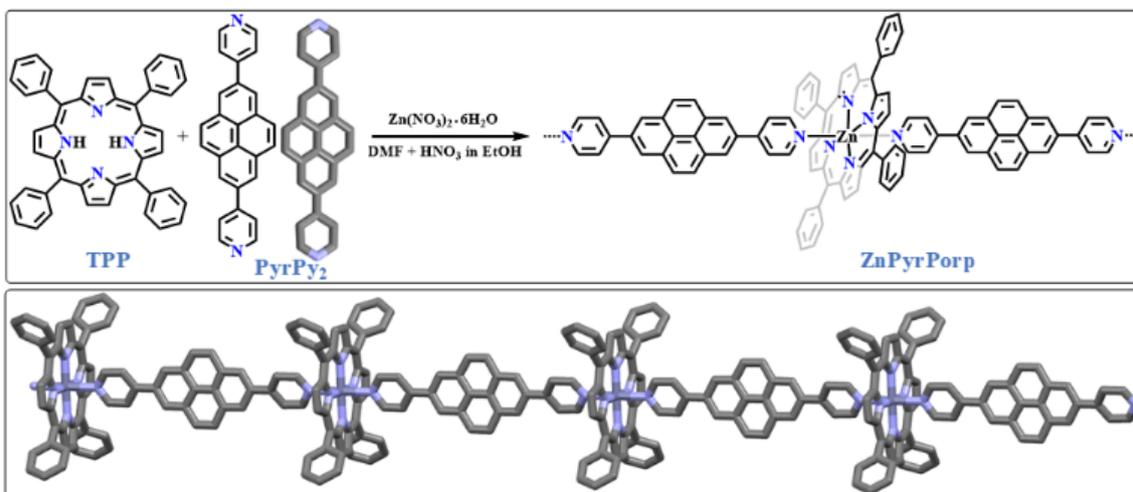
Zoom 4 FRI 16:00~17:00

Zinc-Pyrene Porphyrin 1-D-Polymer based Photocatalyst

Gajendra Gupta, Miyeon Kim, Chang Yeon Lee*

Department of Energy and Chemical Engineering, Incheon National University, Korea

Among metal organic materials, coordination polymers with 1-D architectures have received considerable interests due to their aesthetic molecular structures and applications in various important fields. However, synthesizing polymers at 1-D level with absolute precision is difficult due to the presence of several coordination sites from the metal source and the bridging ligands, which often lead to the formation of 2-D or 3-D polymers. Porphyrin and pyrene are two important widely used chromophores in metal organic synthesis with broad and significant applications. Herein, we present the synthesis of a zinc metal based pyrene-porphyrin hybrid linear 1-D coordination polymer synthesized through a facile one-pot solvothermal process. The single crystal X-ray structure shows an interesting morphology with zinc metal coordinated to the porphyrin center which is further connected to the pyrene ligands forming an interesting 1-D-type polymer. The photophysical properties of the polymer were studied in detail. The polymer has the ability to harvest light as confirmed by time correlated single photon counting and confocal laser scanning microscopy studies. In addition, it also showed excellent catalytic activity towards photooxidation of 1,5-dihydroxynaphthalene (DHN) to 5-hydroxy-1,4-naphthaquinone (Juglone). Figure : Scheme showing the formation of ZnPyrPorp polymer and its SCXRD structure.



Poster Presentation : **INOR.P-163**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Toward New Ferrocene Derivatives Stabilized by N-heterocyclic Carbenes (NHCs) for Redox-active Materials

Hyeonjeong Choi

Chemistry, Pohang University of Science and Technology, Korea

Reduction of Fe(II)-ferrocene (Fc) derivatives is well-known to decompose because their radical structures are unstable. Nevertheless, we successfully demonstrated that the reduced structures of ferrocene derivatives could be stabilized by π -accepting ability of NHC ligands. From the discovery, we further applied Fc-NHC molecules as redox-active organic materials (ROMs) to the redox flow batteries (RFBs) system. RFBs are considered one of the most promising energy storage systems (ESSs) because they can generate renewable energy and have great scalability and flexibility. Therefore, many researchers have been developing more efficient RFBs systems. In this work, a new class of ROMs is described for non-aqueous RFBs. Various NHC-based ferrocene derivatives are successfully synthesized and their redox chemistry was investigated. More detailed studies will be presented.

Poster Presentation : **INOR.P-164**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Hollow nanostructure of ternary ordered alloy for oxygen reduction electrocatalyst

YunChang Son, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Improving the activity and durability of electrocatalysts for sluggish oxygen reduction reaction(ORR) has been the most critical and essential task in fuel cell technologies. Hollow Pt-based bimetallic nanostructures such as nanoframes and nanocages have received great attention due to their excellent ORR activity, benefited from their high surface area. However, their low electrocatalytic durability caused by the electrochemical dealloying of non-Pt element is one of the critical hurdles for practical application in fuel cell devices. Meanwhile, formation of Pt-based ternary alloy or atomically-ordered intermetallic alloy could improve the ORR durability due to suppressed dealloying under electrocatalytic condition, which is originated from high phase stability with strong orbital interaction. However, the phase transition process from random alloy to intermetallic phase requires high temperature, which collapses the structural feature. Herein, we report the protective-layer assisted synthesis of hollow structured, ternary Pt-based electrocatalysts possessing atomically-ordered alloy phases. The protective layer prevents the collapse of the hollow morphology during thermal annealing process. Ternary intermetallic Pt-based hollow nanostructure exhibited enhanced ORR activity and durability due to their high surface area and improved phase stability.

Poster Presentation : **INOR.P-165**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Indol-2-ylidene (IdY): Ambiphilic N-heterocyclic carbene derived from indole

Hyunho Kim, Minseop Kim¹, 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*

Cyclic (alkyl)(amino)carbenes (CAACs) are receiving remarkable attention because of their ambiphilic properties. The formal replacement of one nitrogen atom (π -electron donating, σ -withdrawing) by an alkyl group (σ -donating) makes these carbenes more electrophilic 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. Following the pioneering work on CAACs, other classes of ambiphilic NHCs have been developed such as cyclic (amino)(aryl)carbenes (CAArCs). Ambiphilicity of CAArCs could be increased by replacing the amino group with an aryl group. 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. Moreover, because the indole motif is one of the most common N-heterocycles found in drug molecules and natural products numerous synthetic methods for the indole moiety have been reported to date. Herein, the synthesis of indole derived ambiphilic N-heterocyclic carbene ligand, indol-2-ylidene (IdY), is described. A series of indolenium precursors were prepared on a gram scale in good yields. Trapping experiments with elemental selenium, $[\text{RhCl}(\text{cod})]_2$ and CuCl provided the expected carbene adducts. Further computational and spectroscopic studies supported the ambiphilicity of IdY, which lies between cyclic (alkyl)(amino)carbenes (CAAC-5) and cyclic (amino)(aryl)carbene (CAArC). The copper complexes show high percent buried volume ($\%V_{\text{bur}} = 58.1$) and allow for carboboration of terminal alkynes within 30 minutes in a demonstration of synthetic utility with good yields and high regioselectivity. Further development of the IdY framework for free carbene isolation is currently underway in our laboratory and will be reported in due course.

Poster Presentation : **INOR.P-166**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Synthesis of Pd₃Pb Nanosponges as Catalysts for the Conversion of Furfural

Minki Jun, Dongyong Kim, Heejin Kim, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Furfural (FAL) is a kind of abundant biomass obtained by dehydration reaction of xylose from peanut husks, cornstalks, and many other agricultural wastes. Among the various kinds of furfural downstream products, furfuryl alcohol (FOL) is one of the most important chemicals because it is widely used as an intermediate for producing useful compounds such as lysine, vitamin C, lubricants, and resins. Therefore, it is crucial to develop a catalyst that facilitates the reaction kinetics in the hydrogenation of FAL and exhibits high selectivity for the FOL. Herein, we report the synthesis of sponge-like Pd₃Pb multiframe (Pd₃Pb MFs) as catalysts for the hydrogenation of FAL. The prepared Pd₃Pb MFs exhibit superior activity and selectivity for the hydrogenation of FAL to FOL.

Poster Presentation : **INOR.P-167**

Inorganic Chemistry

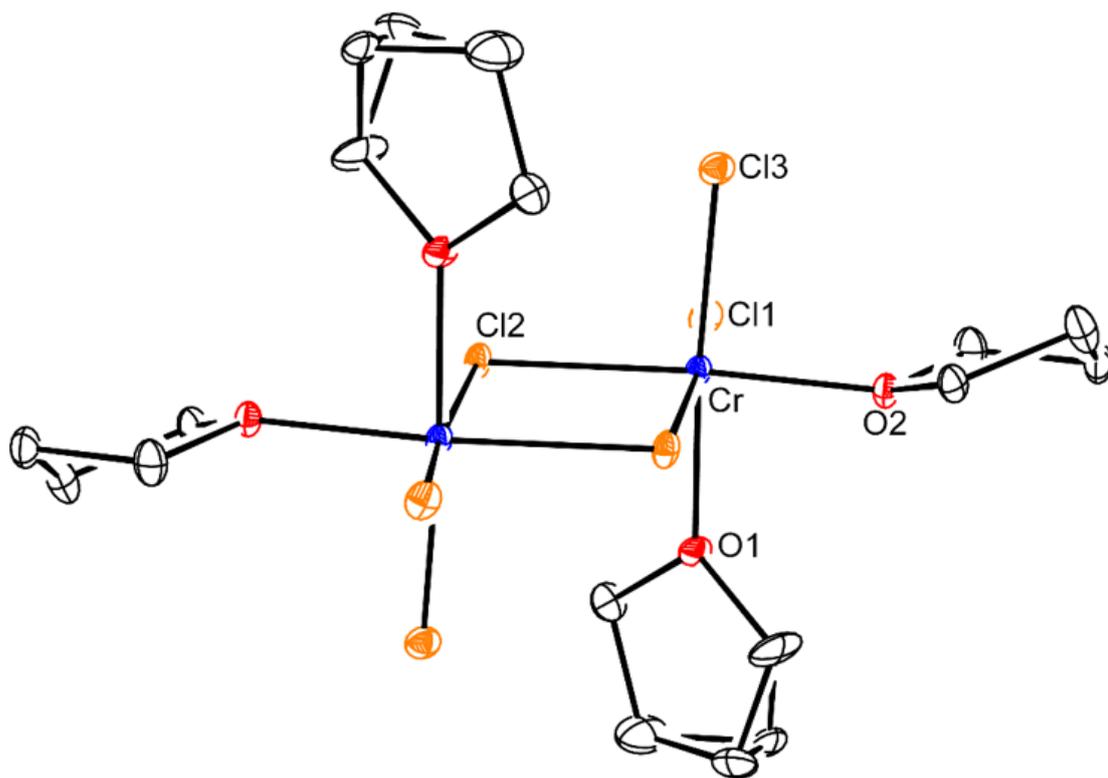
Zoom 4 FRI 16:00~17:00

Well-Defined $[\text{CrCl}_2(\mu\text{-Cl})(\text{thf})_2]_2$ for Replacing the Common Chromium Source $\text{CrCl}_3(\text{thf})_3$

DongGeun Lee, Bun Yeoul Lee*

Department of Molecular Science and Technology, Ajou University, Korea

$\text{CrCl}_3(\text{thf})_3$ is a common starting material in the synthesis of organometallic and coordination compounds of Cr. However, it caused problems in some cases because it is not a purity guaranteed chemical that deposited as an irregular solid with no possibility of recrystallization. In this work, we synthesize a well-defined form of the THF adduct of CrCl_3 ($[\text{CrCl}_2(\mu\text{-Cl})(\text{thf})_2]_2$), a crystalline solid, that enables structure determination by X-ray crystallography. Moreover, its preparation procedure is facile: evacuation of $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ at 100 °C, treatment with 6 eq Me_3SiCl in a minimal amount of THF, and crystallization in CH_2Cl_2 . A reliably high activity (6600 kg/g-Cr/h; 1-octene selectivity at 40 °C, 75%) was exhibited when the ethylene tetramerization catalyst $[\text{iPrN}\{\text{P}(\text{C}_6\text{H}_4\text{-}p\text{-Si}(\text{nBu})_3)_2\}_2\text{CrCl}_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ was prepared using well-defined $[\text{CrCl}_2(\mu\text{-Cl})(\text{thf})_2]_2$ as a starting material, while that of the one prepared using the impure $\text{CrCl}_3(\text{thf})_3$ was inconsistent and relatively low (~3000 kg/g-Cr/h). By using well-defined $[\text{CrCl}_2(\mu\text{-Cl})(\text{thf})_2]_2$ as a Cr source, single crystals of $[(\text{CH}_3\text{CN})_4\text{CrCl}_2]^+[\text{B}(\text{C}_6\text{F}_5)_4]^-$ and $[\{\text{Et}(\text{Cl})\text{Al}(\text{N}(\text{iPr})_2)_2\}\text{Cr}(\mu\text{-Cl})_2]$ were obtained, allowing structure determination by X-ray crystallography, which had been unsuccessful when the previously known $\text{CrCl}_3(\text{thf})_3$ was used as the Cr source.



Poster Presentation : **INOR.P-168**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Mixed rutile type RuRh oxide nanosandwiches as highly active and stable electrocatalyst toward the oxygen evolution reaction

Soo Bean Kim, Jinhyoung Jo, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Since hydrogen production through the electrochemical water-splitting reaction is regarded as a promising pathway to reduce global warming. However, due to its sluggish kinetics of oxygen evolution reaction (OER), searching for highly active and stable catalysts has attracted tremendous interest in the research fields. As ruthenium and ruthenium oxides are well known for their excellent activity, but poor stability due to the fast dissolution during the reaction. Therefore, stabilizing Ru-based nanocatalysts, while maintaining high activity, remains challenging. Herein, we applied rhodium in the ruthenium oxide nanosandwiches, which has the almost similar rutile crystal structure of their oxide species. The mixed-rutile structure was formed through the deposition of Ru on the surface of $\text{Cu}_{2-x}\text{S}@Rh_2\text{S}_3$ hexagonal nanoplates. We found that the RhRu layer with $\text{RhRu}@\text{(RuRh)O}_2$ exhibited great durability with the enhanced activity toward OER

Poster Presentation : **INOR.P-169**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

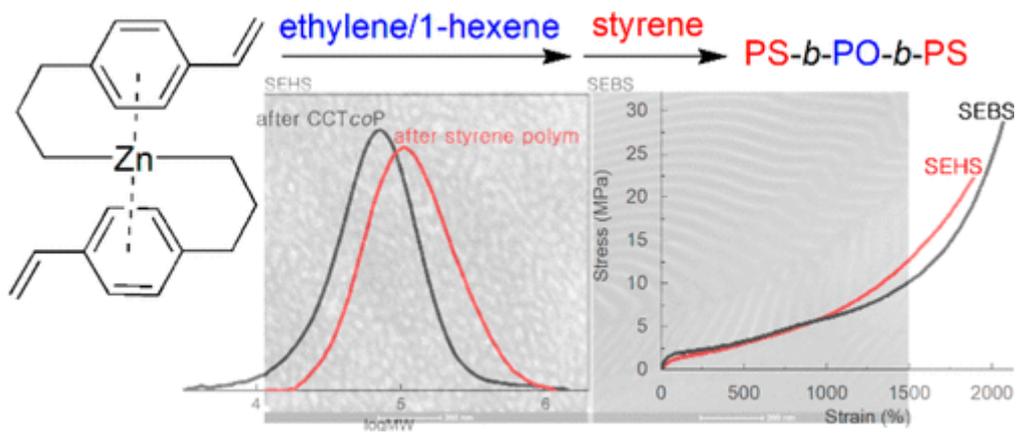
Preparation of Diorganozinc Compounds Carrying Styrene Moieties for Production of Polystyrene-Poly(ethylene-*co*-1-hexene)-Polystyrene Triblock Copolymers

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*

PS-*block*-poly(ethylene-*co*-1-butene)-*block*-PS (SEBS), which is produced via hydrogenation of PS-*block*-polybutadiene-*block*-PS (SBS), is a high performance thermoplastic elastomer used commercially in various areas. The hydrogenation process is costly and tedious being a huddle for market expansion of SEBS. Thus, we envisioned a new one-pot SEBS-like triblock copolymer synthetic scheme to grow PO chains from styrene moiety-carrying diorganozinc compounds by coordinative chain transfer polymerization (CCTP), followed by anionic styrene polymerization using a specially designed initiator, allowing PS chain growth from not only the styrene moieties but also the Zn-C sites. One of the biggest problem in this expedient synthetic scheme is securing a large scale preparation of highly pure diorganozinc compound carrying styrene moieties. The problem was solved in this work by developing synthesis of $(\text{CH}_2=\text{CHC}_6\text{H}_4\text{CH}_2\text{CH}_2\text{CH}_2)_2\text{Zn}$, which is stable and crystalline solid. This enabled the preparation of PS-*block*-poly(ethylene-*co*-1-hexene)-*block*-PS (SEHS), which exhibited a stress-strain curve similar to that of the commercial-grade SEBS. The SEHS dispersed better in a polypropylene (PP) matrix, allowing it to act as a better toughening agent for PP blending than the commercial-grade SEBS. Moreover, SEHS was less viscous, exhibiting better workability.



Poster Presentation : **INOR.P-170**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Environmental Remedy of Pharmaceuticals using Zirconium Metal-Organic Framework

Eunyoung Kang, Hye Jin Cho, David Yang, Seonghun Kim, Joochan Nam, Wonyoung Choe*

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

Water is essential for every living creature. The important element has been contaminated by pharmaceuticals and personal care products such as antibiotics and non-steroidal anti-inflammatory drugs(NSAIDs). The demand for developing an effective purifying material has increased with the rapid increase in drug use. Herein, we demonstrate a study of adsorptive removal for naproxen and ibuprofen, the representative NSAIDs, from an aqueous solution using PCN-224. PCN-224, the highly porous and water-stable metal-organic framework, was solvothermally synthesized and utilized as the effective adsorbent for the target molecules with a carboxylic acid group. We found that the Zr₆ node interacted with the carboxylate moiety of the two targets exhibiting nearly 100% removal efficiency. PCN-224 removed less than 40 % of targets without the specific functional group with respect to the surface area and porosity. Therefore, PCN-224 is suggested as a competitive adsorbent, especially for the drugs embracing carboxylic acids, such as naproxen and ibuprofen.

Poster Presentation : **INOR.P-171**

Inorganic Chemistry

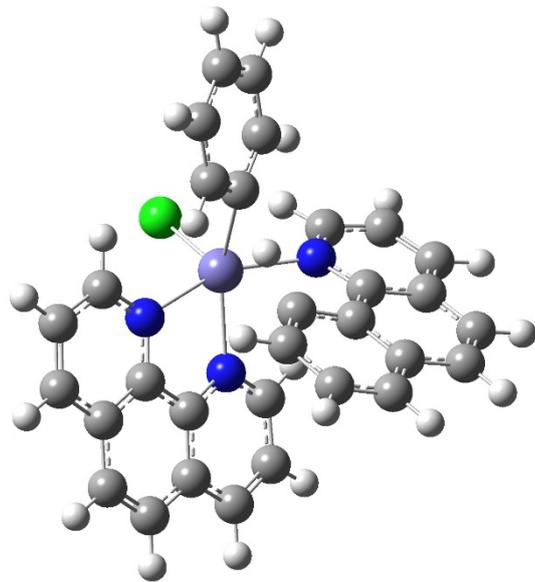
Zoom 4 FRI 16:00~17:00

Linear free energy relation in spin-dependent C-H bond activation by iron-complexes

Yongho Kim^{*}, SoHyeon Lee

Department of Applied Chemistry, Kyung Hee University, Korea

Density functional theory (DFT) calculations were used to study the structure-activity relation in C-H bond activation by iron complexes. The C-H arylation by iron-complex has been proposed to occur by a two-state reactivity scenario in which the low-spin Fe(II) singlet state crosses over the high-spin ground state and promotes C-H bond cleavage. Electron-donating and withdrawing substituents were introduced to benzo[h]quinoline ligand of iron complexes and the spin-dependent free energies were calculated depending on the position. A good linear relation between reaction and activation free energies was observed, however, the slope depend greatly on the position of the substituent. We found the the electron-withdrawing substituent lowers the activation energies, which implies that a new and better catalyst can be made by introducing an electron-withdrawing group in benzo[h]quinoline ligand.



Poster Presentation : **INOR.P-172**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Synthesis and Structural Analysis of 1-D Zinc Tetrazole Coordination Polymer

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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. 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 ($\kappa^3\text{-O3}$, $\kappa^3\text{-N3}$), 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.

Poster Presentation : **INOR.P-173**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Theoretical Perspectives in IdY-Grubbs Catalysts

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

Electronic and steric properties of N-heterocyclic carbene (NHC) ligands are crucial factors for many transition metal catalysis including Grubbs catalyst in olefin metathesis. Numerous NHCs have been successfully introduced to Grubbs catalysts such as 5-membered or 6-membered cyclic (alkyl) amino carbene (cAAC), diamidocarbene (DAC), and abnormal NHCs. Among these, cAACs ligated Grubbs catalysts have attracted great attention because cAACs can stabilize the ruthenium complex and cAACs ligated Grubbs catalysts show remarkable reactivity in ethenolysis. In 2020, our group designed a new type of NHC, indol-2-ylidene (IdY), which was derived from indole structures. IdYs can tune their electronic properties and steric properties by changing aromatic substituents. Experimental data (⁷⁷Se NMR and Tolman Electronic Parameter value) showed that IdY's electronic properties can be tuned in a wide range and show strong electrophilic property. In addition, IdYs can also support transition metal ions such as rhodium and copper metal ions. Herein, we designed IdY-Grubbs catalysts. By DFT calculation, we also discovered that the HOMO and LUMO energies of IdY-Grubbs catalysts change in the right direction, as demonstrated by Togni and Sigman groups.

Poster Presentation : **INOR.P-174**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Selective Synthesis of Iridium Supramolecules Using Tetrazolyl Ligands

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Dative coordination bonding between metal center and electron donor like pyridine and imidazole 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. In the field of coordination chemistry, a variety of mon-, di- or tri-tetrazolyl systems have been used as linkers for the complexation. For example, platinum and palladium complexes containing monodentate tetrazolyl units have been reported. Also, there have been several interesting reports on the multinuclear metal complexes containing bridging tetrazole ligands. However, the examples of the complexes possessing chelating tetrazolyl ligands are relatively sparse. Only limited examples of octahedral iridium(III) complexes have been reported recently as very strong luminescent materials. Our group is interested in the chelate tetrazolyl system and is trying to synthesize several supramolecules using the iridium metal. Herein, we report the selective synthesis of multinuclear iridium supramolecules having different shapes by means of the binding mode control of tetrazole ligands. By controlling the reaction condition, different ligations of tetrazolyl ligands were achieved. Whereas tetrazolyl ligand acted as a chelate ligand at room temperature, bridging mode of tetrazolyl units were observed at high temperature (> 70°C). By using chelating mode, monomeric, dimeric and tetrameric and hexameric iridium complexes were achieved selectively and characterized with various methods including X-ray crystallography. When tetrazole was used as a bridging unit, number of bridging units was modulated by the control of stoichiometry of tetrazole unit and iridium dimer, resulting in the formation of dinuclear iridium complexes containing one, two or three bridging tetrazolyl units. By using pyridyl tetrazole, interesting pyridine electron donors were obtained and they were used in the self-assembly of various polygons.

Poster Presentation : **INOR.P-175**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Axial Ligand Dependent Reactivity of C-H Bond Activation by Cpd-I and the Role of Spin Density Distribution

Yooncheol Choi, Yongho Kim*

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Cytochrome P450 is a catalyst that assist transferring oxygen atom in the nature. In this work, we investigated the reactivity of C-H bond activation depending on axial ligand using density functional theory (DFT) calculations and natural bond analysis. The donor-acceptor interactions of natural orbitals suggest that there is no direct orbital interaction between reaction center of C-H bond cleavage and the axial-ligands. The axial-ligand orbitals interact with the orbitals of phophyrin, which interact with those of Fe-oxo group. These results mean that the axial-ligand dependent reactivity results from an indirect or a secondary effect. Two-state reactivity (TSR) model has been suggested to play an important role to this reaction. The relation between barrier height and the spin density distribution depending on the DFT functionals will be discussed.

Poster Presentation : **INOR.P-176**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

The chemical separation of niobium in simulated radioactive wastes for a radiometric measurement of niobium-94

Kyungwon Suh

Korea Atomic Energy Research Institute, Korea

⁹⁴Niobium(Nb-94) is produced by neutron fission of uranium and plutonium and is also generated by neutron activation reaction of stable niobium by $^{93}\text{Nb}(n,\gamma)^{94}\text{Nb}$. It decays to the excited state of molybdenum-94 by the emission of beta particles, and this excited state decays to stable molybdenum-94 by emission of gamma rays. It is a long-lived radionuclide and so it is very critical to quantify the amount of Nb-94 prior to permanent disposal of radioactive wastes. Although it is a gamma-emitting radionuclide, it can be interfered with co-existing radionuclides such as other beta-gamma emitters. Therefore, a chemical separation is required for a more precise determination of niobium before a radiometric measurement using gamma-detector. To the best of our knowledge, there are several methods available for niobium separation like ion-exchange chromatography, precipitation technique, solvent extraction, extraction chromatography, and integrated test methods. Precipitation technique is a classical and simple method to separate analyte. However, trace niobium is well-known to be co-precipitated as metal hydroxide precipitate with the iron in metallic radioactive wastes like stainless-steel or nickel-based alloys. So, it requires to conduct an additional method for purification of the sample. Herein, I present the result of the separation of niobium in stainless steels and nickel-based alloys. It was confirmed that niobium was quantitatively recovered by the combination of precipitation technique with 10% NH₄OH and MIBK extraction, while the niobium in nickel-based alloys was selectively separated with ion-exchange chromatography instead of the above method.

Poster Presentation : **INOR.P-177**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

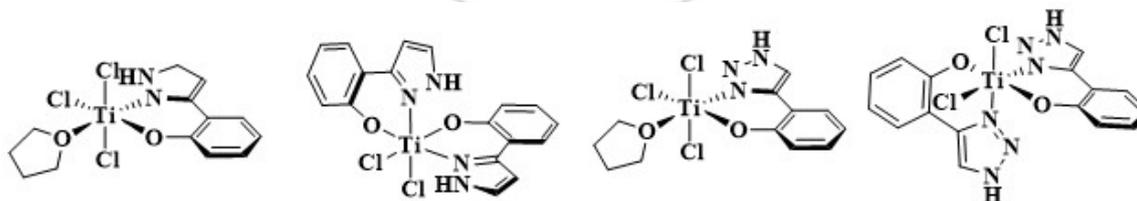
Synthesis of New Titanium(IV) Complexes for carbon dioxide utilization using N-Heterocyclic ligands

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Carbon dioxide emissions are causing serious environmental problems, and the storage and utilization of carbon is being developed day by day to minimize them. Many research groups have focused on the synthesis of cyclic carbonate from the cycloaddition reaction between CO₂ and epoxides. Cyclic carbonate obtained from CO₂ cycloaddition reaction is known as a high value-added product, such as organic solvents and electrolytes in secondary batteries. We previously reported the synthesis of titanium complexes using tetrazolyl ligands and their high activities in the cycloaddition reaction of CO₂. To investigate the role of tetrazolyl group in the catalysis, various titanium complexes possessing azole ligands such as pyrazole and triazole have been prepared and used in CO₂ cycloaddition reactions. In this study, detailed synthetic routes of complexes and the catalytic properties of them are presented and discussed



Poster Presentation : **INOR.P-178**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Experimental and Theoretical Studies for the Zintl Thermoelectric $\text{Ca}_{3-x}\text{Yb}_x\text{AlSb}_3$ System

Yeongjin Hong, Tae-Soo You*

Department of Chemistry, Chungbuk National 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: $\text{A}_{14}\text{MSb}_{11}$ ($\text{A} = \text{Ca}, \text{Yb}$; $\text{M} = \text{Mn}, \text{Al}$), $\text{A}_5\text{Al}_2\text{Sb}_6$ ($\text{A} = \text{Ca}, \text{Yb}$), $\text{A}_{11}\text{Pn}_{10}$ ($\text{A} = \text{Ca}, \text{Yb}$; $\text{Pn} = \text{Sb}, \text{Bi}, \text{Sn}$), A_2CdSb_2 ($\text{A} = \text{Ca}, \text{Yb}, \text{Eu}$), and A_3MSb_3 ($\text{A} = \text{Ca}, \text{Sr}$; $\text{M} = \text{Al}, \text{Ga}$) series. Among the Zintl phase thermoelectric compounds, the A_3MPn_3 ($\text{A} = \text{Ca}, \text{Sr}, \text{Ba}, \text{Eu}$; $\text{M} = \text{Al}, \text{Ga}, \text{In}$; $\text{Pn} = \text{Sb}, \text{As}, \text{P}$) 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 (*P2₁/c*), Rb_3TiO_3 (*P2₁/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 $\text{Ca}_{3-x}\text{Yb}_x\text{AlSb}_3$ ($0 \leq x \leq 0.82(2)$) is consist of three compound as Ca_3AlSb_3 (loaded composition $\text{Ca}_3\text{AlSb}_{2.7}\text{Ge}_{0.3}$), $\text{Ca}_{2.59(2)}\text{Yb}_{0.41}\text{AlSb}_3$, $\text{Ca}_{2.18(2)}\text{Yb}_{0.82}\text{AlSb}_3$. These compounds were synthesized by the arc-melting method, and their crystal structures were characterized by both powder and single-crystal X-ray diffractions. Dopants including Yb, Ge in the $\text{Ca}_{3-x}\text{Yb}_x\text{AlSb}_3$ system is Ca-rich compound. Quite interestingly, $\text{Ca}_{3-x}\text{Yb}_x\text{AlSb}_3$ initially crystallized in the mixed-phase, but after post-heat treatment, those were converted to the orthorhombic *Pnma* space group ($Z = 4$, Pearson Code *oP28*) 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 $\text{Ca}_{2.59(2)}\text{Yb}_{0.41}\text{AlSb}_3$, which was quite close to the SXRD result. The thermal stability of $\text{Ca}_{2.59(2)}\text{Yb}_{0.41}\text{AlSb}_3$

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-179**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Effect of cation substitution of the Zintl Thermoelectric $\text{Ca}_{3-x}\text{M}_x\text{AlSb}_3$ ($\text{M} = \text{Sr}, \text{Eu}$) System

Tae-Soo You^{*}, Yeongjin Hong

Department of Chemistry, Chungbuk National 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: $\text{A}_{14}\text{MSb}_{11}$ ($\text{A} = \text{Ca}, \text{Yb}$; $\text{M} = \text{Mn}, \text{Al}$), $\text{A}_5\text{Al}_2\text{Sb}_6$ ($\text{A} = \text{Ca}, \text{Yb}$), $\text{A}_{11}\text{Pn}_{10}$ ($\text{A} = \text{Ca}, \text{Yb}$; $\text{Pn} = \text{Sb}, \text{Bi}, \text{Sn}$), A_2CdSb_2 ($\text{A} = \text{Ca}, \text{Yb}, \text{Eu}$), and A_3MSb_3 ($\text{A} = \text{Ca}, \text{Sr}$; $\text{M} = \text{Al}, \text{Ga}$) series. Among the Zintl phase thermoelectric compounds, the A_3MPn_3 ($\text{A} = \text{Ca}, \text{Sr}, \text{Ba}, \text{Eu}$; $\text{M} = \text{Al}, \text{Ga}, \text{In}$; $\text{Pn} = \text{Sb}, \text{As}, \text{P}$) 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 (*P2₁/c*), Rb_3TiO_3 (*P2₁/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 $\text{Ca}_{3-x}\text{M}_x\text{AlSb}_3$ ($\text{M} = \text{Sr}, \text{Eu}$; $0 \leq x \leq 0.58(2)$) is consist of three compound as Ca_3AlSb_3 (loaded composition $\text{Ca}_3\text{AlSb}_{2.7}\text{Ge}_{0.3}$), $\text{Ca}_{2.48(2)}\text{Sr}_{0.52}\text{AlSb}_3$, $\text{Ca}_{2.42(1)}\text{Eu}_{0.58}\text{AlSb}_3$. These compounds were synthesized by the arc-melting method, and their crystal structures were characterized by both powder and single-crystal X-ray diffractions. The $\text{Ca}_{3-x}\text{M}_x\text{AlSb}_{3-y}\text{Ge}_y$ system is a Ca-rich compound in which Eu and Sr are substituted to Ca, which is a cation, and Ge is doped to Sb, which is an anion. $\text{Ca}_{3-x}\text{M}_x\text{AlSb}_{3-y}\text{Ge}_y$ initially crystallized into a mixed-phase, but successfully transformed to a Ca_3AlSb_3 crystal structure after the annealing process. However, Ge is not included as a *p*-type dopant. Also, the observed site preference of cations was investigated using the size-factor criterion, as judged by a volumetric comparison of the central cation and the volume of coordination polyhedra. 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 band structure analyses were thoroughly conducted. In particular, in the case of Ca and Eu mixed compound, the overlap of the conduction band and valence band is confirmed, whereas in the case of Ca and Sr mixed

compound, a slight band gap appeared, which was confirmed to have relative semiconductivity property behavior.



Poster Presentation : **INOR.P-180**

Inorganic Chemistry

Zoom 4 FRI 16:00~17:00

Influence of the *p*-type Double Dopants for the Thermoelectric Properties of the $\text{Ca}_{11-x}\text{A}_x\text{Sb}_{10-y}\text{Ge}_z$, (A = Na, Li) System

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We recently reported the effects of multi-substitution for the thermoelectric (TE) performance in the $\text{Ca}_{11-x}\text{Yb}_x\text{Sb}_{10-y}\text{Ge}_z$ ($0 \leq x \leq 9$; $0 \leq y \leq 3$; $0 \leq z \leq 3$) system. In that study, we exploited the two-track strategy using two different *p*-type substitutions: (1) the cationic Yb mixing for Ca and (2) the anionic Ge doping for Sb, and the influence these multi-substitutions for electronic structures as well as TE performance were thoroughly studied. In order to further expand this series of multi-substituted *p*-type Zintl TE materials, we investigated the double *p*-type doping using both the cation and anion sites in the $\text{Ca}_{11-x}\text{A}_x\text{Sb}_{10-y}\text{Ge}_z$, (A = Na, Li; $0.06(3) \leq x \leq 0.17(5)$; $0.19(1) \leq y \leq 0.72(1)$, $0.22(1) \leq z \leq 0.45(1)$) system. In this work, instead of introducing a single cationic dopant, we respectively introduced two different monovalent cations, Li and Na, along with the anionic Ge dopant. Two title compounds in the $\text{Ca}_{11-x}\text{A}_x\text{Sb}_{10-y}\text{Ge}_z$ system have been synthesized by arc-melting and lead flux synthesis, and characterized by both powder and single-crystal X-ray diffractions. They crystallized in the isotypic $\text{Ho}_{11}\text{Ge}_{10}$ -type structure (tetragonal space group $I4/mmm$, Pearson symbol $tI84$) with nine crystallographically atomic positions in each unit cell, which include one $\text{Ca}^{2+}/\text{M}^+$ mixed-cationic site and one Sb/Ge mixed-anion site. The overall crystal structure can be described as an assembly of three different types of co-facial polyhedra formed by $\text{Ca}^{2+}/\text{M}^+$, which of each is centered by isolated Sb atoms. The 3-D anionic framework can be considered as an assembly of the dumbbell- and square-shaped Sb atoms. The $\text{Ca}_{11-x}\text{A}_x\text{Sb}_{10-y}\text{Ge}_z$ has high crystallinity, forming visible crystals even under the facile arc-melting method. Fully grown octahedral crystals were formed under lead flux synthesis. The different shapes of crystals under different synthesis methods suggest the octahedral crystal is the thermodynamically stable shape, whereas the unique texture of the crystal yielded from arc-melting is the kinetically stable shape. The crystal growth was further investigated via Sn doping. With the same condition as Ge doping, Sn doped product produced more octahedral crystals. This is due to Sn having less size difference from Sb, thus being able to occupy more of the Sb3 site and removing electrons while lessening

the Sb₃ vacancy. To further investigate the overall electronic structure and chemical bonding in the title compounds, a series of DFT calculations using the TB-LMTO-ASA method were performed for two hypothetical structural models of Ca_{10.5}M_{0.5}Sb_{9.5}Ge_{0.5} (M = Li, Na). In addition, DOS, COHP, ELF, and band structures were also calculated. The series of TE property measurements are underway.



Poster Presentation : **INOR.P-181**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Effect of Cationic and Anionic Doping in the Quinary Zintl Phase Thermoelectric Material $\text{Ca}_{5-x}\text{Yb}_x\text{Al}_{2-y}\text{In}_y\text{Sb}_{6-z}\text{Sn}_z$ System

Junsu Lee, Tae-Soo You*

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Recent research results show that the carrier mobility of the $\text{Ca}_5\text{Al}_{2-x}\text{In}_x\text{Sb}_6$ system can be increased by the In-substitution for Al. In addition, the Zn-doping for the Al/In-mixture in the $\text{Ca}_5\text{Al}_{1.9-x}\text{In}_x\text{Zn}_{0.1}\text{Sb}_6$ system further improved the carrier concentration and eventually resulted in the enhancement of electrical conductivities. Furthermore, the lattice thermal conductivity decreased due to the increased phonon scattering by the Al/In-mixing along with the Zn-doping. Therefore, these combined effects eventually improved the ZT of the compounds in this system. In this research, we discuss our attempts to introduce the cationic Yb-substitution for Ca and the anionic p -type Sn-doping for Sb in the Al/In-mixed $\text{Ca}_{5-x}\text{Yb}_x\text{Al}_{2-y}\text{In}_y\text{Sb}_{6-z}\text{Sn}_z$ system. The title compounds were successfully synthesized by arc-melting and characterized by both powder and single-crystal X-ray diffractions. In particular, $\text{Ca}_{1.02}\text{Yb}_{3.98}\text{Al}_{1.48}\text{In}_{0.52}\text{Sb}_6$ with the Ca/Yb-mixture showed the phase-transition from its original $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type to the $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type phase after the post-heat-treatment, whereas $\text{Ca}_5\text{Al}_{1.73}\text{In}_{0.27}\text{Sb}_{5.44}\text{Sn}_{0.56}$ with only the Ca cation maintained its original $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type phase before and after the annealing process. Both two title structures of the $\text{Ba}_5\text{Al}_2\text{Bi}_6$ -type and $\text{Ca}_5\text{Ga}_2\text{Sb}_6$ -type phases adopt the orthorhombic space group $Pbam$ ($Z = 2$, $oP26$) with a total of seven independent atomic sites, including three Ca sites, three Sb sites, and one Al sites in a unit cell. The site-preference of cationic Ca and Yb can be rationalized by the size-factor criterion, while that of anionic Sb and Sn should be elucidated by the electronic-factor criterion. A series of DFT calculations using the tight-binding linear muffin-tin orbital (TB-LMTO) method was performed, and the resultant density of states (DOS) and band structures were thoroughly investigated to understand the effect of p -type Sn-doping on the electrical transport property.

Poster Presentation : **INOR.P-182**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Ru-based mixed metal oxide to enhance the activity in acidic oxygen evolution reaction via pyrolysis

Jinhyoung Jo, Kwangyeol Lee*

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Electrocatalysts driving oxygen evolution reaction (OER) in acidic electrolytes are highly needed to overcome the sluggish kinetics caused by the four electrons and four proton-coupled reactions, and thus to reduce the large overpotential associated with overall water splitting. Currently, Ru-based catalysts have been spotlighted as a promising candidate among the anodic materials for the commercial water electrolyzer due to their higher activity than Ir-based catalysts toward the oxygen evolution reaction (OER). However, increasing their stability still remains challenging to date. For overcoming this challenge, approaches such as mixed metal oxide frameworks, which are doped Ru atoms, have been used as alternative strategies in designing robust OER electrocatalysts. In this work, we show the synthetic strategy for mixing RuO₂ and lead oxide to enhance the catalytic stability via annealing and electrochemical processes. The mixing of Ru with the metal oxide supports might boost the sluggish kinetics of OER and alleviate the degradation of Ru-based electrocatalysts in acidic electrolytes. We prepare the RuO₂/Ru-doped PbO_x-based nanocluster/nanocube heterostructures from the hetero-interfaces between the Ru cluster and the PbS nanocubes through the pyrolysis in the air and sequential electrochemical process. These RuO₂/Ru-doped PbO_x-based nanocluster/nanocube heterostructures exhibit great activity and stability towards the acidic OER. From this work, we expect that the appropriate electrochemical condition can control Ru dopant in the PbO_x, and thus allow to optimize activity and stability toward the acidic OER.

Poster Presentation : **INOR.P-183**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Pd@COF-QA: a phase transfer composite catalyst for aqueous Suzuki–Miyaura coupling reaction

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Although covalent organic frameworks (COFs) are in their early teens, as a typical class of organic crystalline porous species, they have already shown promise as functional materials in gas adsorption, separation, proton conduction, optical devices, drug delivery, chemical sensing, energy storage, and catalysis. Phase-transfer catalysis (PTC) is a promising green technique for organic transformation due to its simple operation, aqueous medium and mild reaction conditions. A series of MOF-based PTC catalytic systems which are good promoters of organic transformations in the aqueous phase. As promising alternatives to MOFs, the covalent bond driven COFs should be more stable in the aqueous phase, and their PTC behaviour is really worth pursuing. Herein, we report a Pd NP-loaded and N,N-dimethyldodecyl ammonium bromide-decorated COF. The obtained Pd@COF-QA and its chitosan aerogel-based continuous flowthrough reactor can be used as an excellent phase transfer catalyst to promote the Suzuki–Miyaura coupling reaction in water under mild conditions even at a gram scale.



Poster Presentation : **INOR.P-184**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Chain Connectivity of Metallic, Coordinative, and Hydrogen Bonds in a Paddlewheel Metal-Organic Framework HKUST-1

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Hydrogen bond (HB) is one of the most intensively studied subject in contemporary science, including chemistry, biology, physics, and environmental science because the HB has shown various behavior depending on molecular conditions such as its phase, surrounding molecules, temperature, and pressure. Nevertheless, HB confined in nanocage has been rarely studied. Metal-organic frameworks (MOFs) are a class of highly crystalline porous materials that are constructed by the continuous links of metal ions and multivalent organic ligands. Their high porosity, high internal surface area, and chemical functionality have provided numerous opportunities for various applications. Among the MOFs, HKUST-1 (hereafter denoted as HK) that comprises of Cu_2^+ ion and benzenetricarboxylate ligand is a well-known MOF containing paddlewheel Cu-Cu unit. An interesting feature of HK is that all Cu_2^+ ions possess open metal sites that face towards the center of large pores. The second feature is that all Cu_2^+ centers function as Lewis acid that can associate with Lewis base solvent molecules via coordination bond. The third feature is that it possesses Cu-Cu nodes that exhibit stretching vibrational band at the frequencies of 163-230 cm^{-1} depending on the coordination environment around the Cu nodes. Thus, the Raman frequencies of the Cu-Cu vibration reflects the solvent coordination as well as HB associated between the coordinated and pore-filling solvents. In this poster presentation, we show that the presence or absence of HB around the Cu metallic nodes can be monitored by the changes in the frequencies of Cu-Cu vibrational band. Further, we show an interesting property of pore-filling water molecules that behave as zeolitic water.

Poster Presentation : **INOR.P-185**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

A High-Valent Manganese(IV)-Oxo-Ce(IV) Complex and Its Enhanced Oxidizing Reactivity

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A mononuclear nonheme manganese(IV)-oxo complex binding Ce⁴⁺ ion, [(dpaq)Mn^{IV}(O)]⁺-Ce⁴⁺ (**1**-Ce⁴⁺), was synthesized by reacting [(dpaq)Mn^{III}(OH)]⁺ (**2**) with cerium(IV) ammonium nitrate (CAN). **1**-Ce⁴⁺ was well characterized using various spectroscopic techniques, such as UV-vis, EPR, CSI-MS, rRaman, XANES, and EXAFS, showing Mn-O double bond character with a Mn-O bond distance of 1.69 Å and a rRaman band at 675 cm⁻¹. The binding of Ce⁴⁺ ion to the Mn-O moiety was strongly supported not only by the spectroscopic characterization but also by the metal ion-substitution reaction. The one-electron reduction potential of **1**-Ce⁴⁺ was also determined from the electron-transfer reaction. Electron-transfer and oxygen atom transfer reactivities of **1**-Ce⁴⁺ were found to be greater than those of Mn^{IV}(O) intermediates binding redox-inactive metal ions (**1**-Mⁿ⁺). To the best of our knowledge, this study reports the first example of a redox-active Ce⁴⁺ ion-bound Mn(IV)-oxo complex and its spectroscopic characterization and chemical properties (D. G. Karmalkar, M. Sankaralingam, M. S. Seo, R. Ezhov, Y.-M. Lee, Y. N. Pushkar, W.-S. Kim, S. Fukuzumi, W. Nam, *Angew. Chem., Int. Ed.*, **2019**, 58, 16124-16129).

Poster Presentation : **INOR.P-186**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

CsPb(Br/Cl)₃@ZnS core@shell nanocrystals for efficient and stable deep-blue emitting materials

Chung man Yu, Kwangyeol Lee*

Department of Chemistry, Korea University, Korea

Metal halide perovskite nanocrystals (NCs) have shown promising potential in optoelectronic devices due to their excellent optoelectronic properties and tunable emission colors. However, perovskites suffer from poor stability against moisture, light, and heat. Also, the efficiency of blue materials is still lower compared to green and red counterparts. Here, we synthesized the blue-emitting CsPb(Br/Cl)₃@ZnS core@shell NCs by introducing zinc halide and sulfur source. CsPb(Br/Cl)₃@ZnS core@shell NCs show higher water stability and photoluminescence quantum yield than CsPb(Br/Cl)₃ NCs without zinc sulfide shell. This work offers a new strategy for synthesis core@shell heterostructures based on metal halide perovskite NCs.

Poster Presentation : **INOR.P-187**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

***Para*-acridine-appended triarylboron compounds with different boryl acceptors for efficient blue thermally activated delayed fluorescence**

Young Hoon Lee, Hanif Mubarak, Kihoon Shin, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

We report highly efficient blue TADF emitters composed of 9,9-dialkylacridine (9,9-dimethylacridine (DMAC) or 9,9-diphenylacridine (DPAC)) donors (D) and boryl (9-boraanthryl (BA) or dimesitylboryl (BMes₂) acceptors (A). The crystal structures of compounds with the DMAC donor show that the BA ring is almost orthogonal to the phenylene linker, while the BMes₂ unit is tilted by ca 60°. The BA-containing compounds display blue TADF in both the solution and film states. In contrast, BMes₂-containing compounds exhibit normal fluorescence in solution, whereas their films led to blue TADF emission. The doped films of the BA-containing compounds display very short-lived delayed fluorescence of 1.6~2.0 μs, small ΔE_{ST} values below 0.1 eV, and high k_{RISC} of ca. 10^6 s⁻¹. The theoretical and experimental studies support that the BA-containing compounds proceed the stronger charge transfer transition from the donor to the acceptor units than that of the BMes₂-containing compounds. The OLED devices of all compounds show pure to deep blue TADF emissions. In particular, the devices including the DMAC donor exhibit high device performance with a maximum external quantum efficiency (EQE) of 21.3%.

Poster Presentation : **INOR.P-188**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Regulation of heterometal coordinated proteins through the interactions with glycoproteins

Yunha Hwang, Seung Jae Lee*, Dong-Heon Lee

Department of Chemistry and Institute for Molecular Biology and Genetics, Jeonbuk National University, Korea

Concanavalin A (ConA), a lectin protein, has been investigated for its ability to bind to a broad range of pathogens, including microorganisms. Due to the potential value of ConA to diagnostic microbiology, its mechanisms of action have been extensively studied; however, studies have reported different binding affinities due to the formation of different complexes. Monomeric structure of ConA can provide crucial information, as most reported structures are dimers or tetramers. We obtained a monomeric structure of ConA (PDB accession: 5YGM) with a resolution of 1.6 Å, and our analysis revealed that metal coordination was a major cause of the carbohydrate-binding ability. When this structure was superimposed with that of metal-free ConA (apo-ConA), the conformational change in Asn14, a calcium-coordination residue, triggered other carbohydrate-binding residues, including Arg228, Asp208, Tyr12, L99, and Tyr100. This result is significant as it elucidates the mechanisms by which Ca^{2+} is crucial for sugar-binding. The monomeric structure of ConA would be crucial for developing diagnostic tools for detecting carbohydrates. Preliminary reports have proposed that the elimination of Mn^{2+} would not affect sugar-binding affinity, although Ca^{2+} is essential for carbohydrate interaction. This study revealed the sequential mechanisms by which metal coordination affects sugar-binding residues. The positional changes in the sidechain of Asn14, a Ca^{2+} -coordinated residue, were found to trigger conformational changes. This structural analysis provides basic information for the controlling of complex structures of ConA and a specific condition of crystallization indicates possible condition for the designing of diagnostic kit that can recognize pathogens, selectively.

Poster Presentation : **INOR.P-189**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Thermally Activated Delayed Fluorescence Properties of *Nido*-Carborane-Triarylborane Dyads with Sterically Modified Phenylene Linker

Surendran Sujith, Nhi Nguyen Ngoc Tuyet, Ina Nur Istiqomah, Min Hyung Lee*

Department of Chemistry, University of Ulsan, Korea

A family of novel thermally activated delayed fluorescence (TADF) compounds based on *nido*-carborane-appended triarylboranes were prepared and fully characterized. A methyl group is introduced into the 4-position of the phenylene ring bearing the *nido*-carborane (7,8-dicarba-*nido*-undecaborane) cage, i.e., at *ortho* position to the cage, in the PhBMes₂ acceptor moiety of *nido*-carborane-triarylborane dyads (*nido*-1—4). X-ray diffraction analyses of 8-H substituted *nido*-1 reveal the existence of steric congestion around the cage, resulting in a highly twisted connectivity between the cage plane and the Ph ring ($\theta = 85.7^\circ$). All compounds exhibit very small ΔE_{ST} values and thereby strong TADF with long emission lifetimes ($\tau_d = 4.8\text{--}9.7 \mu\text{s}$ in THF) in both THF and PMMA film. Computational studies further demonstrate that *nido*-1—4 form a stable twisted structure with large energy barriers to cage rotation, suggesting that the TADF properties of *nido*-1—4 can be persistently retained even in solution. The details of synthesis and photophysical properties will be presented.

Poster Presentation : **INOR.P-190**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Anticancer Actions of Iron Complex That Induces Impaired Redox Balance for Colorectal Cancer Cells.

Yool Lee, Hyeri Jeon, Hanae Lim, Seungwoo Hong*

Department of Chemistry, Sookmyung Women's University, Korea

The activation and formation of dioxygen is of importance in enzymatic and oxidation chemistry. In the dioxygen chemistry, most of the research has sought to characterize the reactive intermediates such as iron-superoxo, -peroxo, and -oxo species, which are frequently found as key intermediates. However, the use of those reactive intermediates or their starting materials of first-row transition metals as potential candidates of cancer cells by provoking the intracellular ROS disequilibrium has been scarcely endeavored. In this regard, a series of first-row transition metal complexes bearing a picolylamine based water soluble ligand, $[M(\text{HN3O2})]^{2+}$ ($M = \text{Mn}^{2+}, \text{Fe}^{2+}, \text{Co}^{2+}, \text{Cu}^{2+}$; $\text{HN3O2} = 2-(2-(\text{bis}(\text{pyridin-2-ylmethyl})\text{amino})\text{ethoxy})\text{ethanol}$) were synthesized and characterized by various spectroscopic methods including X-ray crystallography and evaluated their dioxygen and reactive oxygen species (ROS) activation reactivity. It was found that among these metal complexes, only iron complex, $[\text{Fe}(\text{HN3O2})(\text{H}_2\text{O})]^{2+}$, is capable of activating dioxygen and hydrogen peroxide and generates ROS species. Upon incubation of these complexes with HCT116 cells, only iron complex induced the cell apoptosis with IC₅₀ value of 24.5 μM ; other metal complexes show negligible anti-proliferative activity. The use of immunocytochemistry combined Western blot analysis strongly supported that the apoptosis occurred via intrinsic pathway (e.g., mitochondrial pathway); in intracellular network, $[\text{Fe}(\text{HN3O2})(\text{H}_2\text{O})]^{2+}$ is susceptible to (i) activate and produce ROS species, (ii) induce the impaired redox balance, and (iii) promote the mitochondrial apoptosis pathway in colorectal cancer cells.

Poster Presentation : **INOR.P-191**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Electronic and geometric structure of a trinuclear C_{2v}-symmetric iron(III) complex

Hyejin Shin, Kil Sik Min*

Department of Chemistry Education, Kyungpook National University, Korea

Trinuclear iron complex, [(Hpmidp/pmidep)Fe₂(NCS)₂Fe(NCS)₂] (1), has been prepared by the reaction of N-(2-pyridylmethyl)iminodipropanol (H₂pmidp), KNCS, and FeSO₄•7H₂O 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 shows 6-coordinated geometric structure. That is, two terminal iron ions are coordinated with Hpmidp-/pmidep²⁻, one oxygen atom of a methoxide ion, and one nitrogen atom of a thiocyanate ion, whereas the central iron ion is bonded with two nitrogen atoms of thiocyanate ions, two oxygen atoms of methoxide ions and two oxygen atoms of Hpmidp-/pmidep²⁻ ligands. To confirm the oxidation states of iron ions we have investigated by using Mössbauer spectrum and also used 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 couplings using SQUID measurements. In this poster, we will present and discuss the synthesis, structure, and physical properties of the iron(III) complex.

Poster Presentation : **INOR.P-192**

Inorganic Chemistry

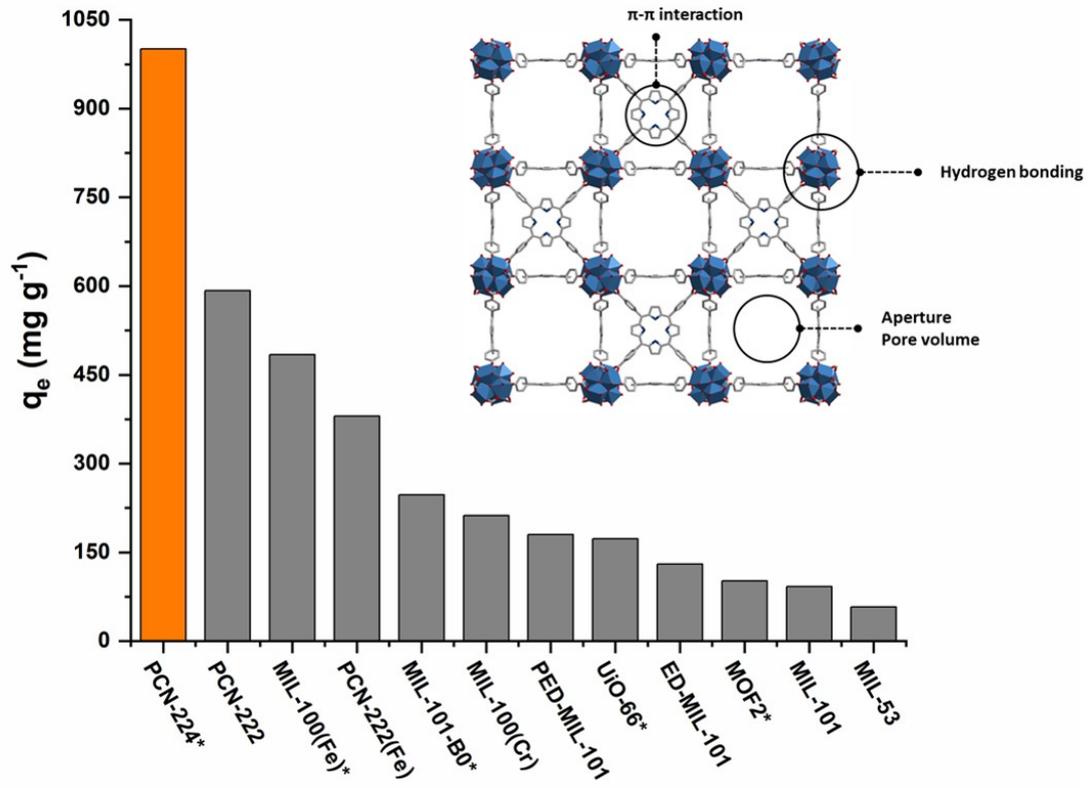
Zoom 5 FRI 15:00~16:00

Enhanced Adsorption removal of Industrial Dyes on Zr porphyrinic Metal-Organic Framework

Eunji Jin, Jiyeon Kim, Joochan Nam, David Yang, Seonghun Kim, Eunyoung Kang, Hye Jin Cho, Wonyoung Choe*

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

Due to anthropogenic activities, fresh water supply is becoming an important issue worldwide. Water sources are often contaminated by industrial dyes and may cause harmful health effects even in low-level exposure. In this work, we present adsorptive removal of representative industrial dyes using PCN-224, known as Zr porphyrinic metal-organic framework. PCN-224 has structural properties such as optimal pore aperture and large pore volume, incorporating dye molecules. Furthermore, various sites such as porphyrin linker and Zr6 node in the structure induce π - π interaction and hydrogen bonding between the framework and organic dye and help to exhibit high adsorption capacity. The results show that PCN-224 exhibits high performance for dye adsorption among reported MOFs.



Poster Presentation : **INOR.P-193**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

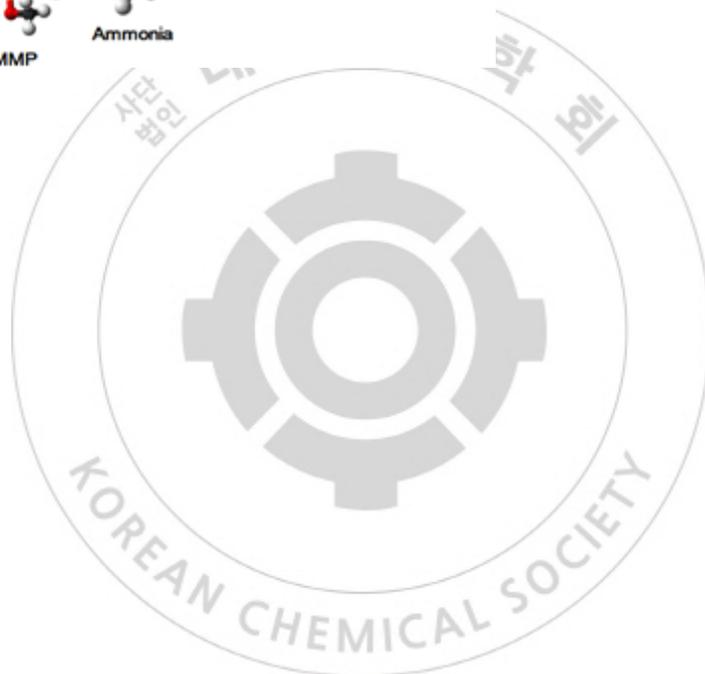
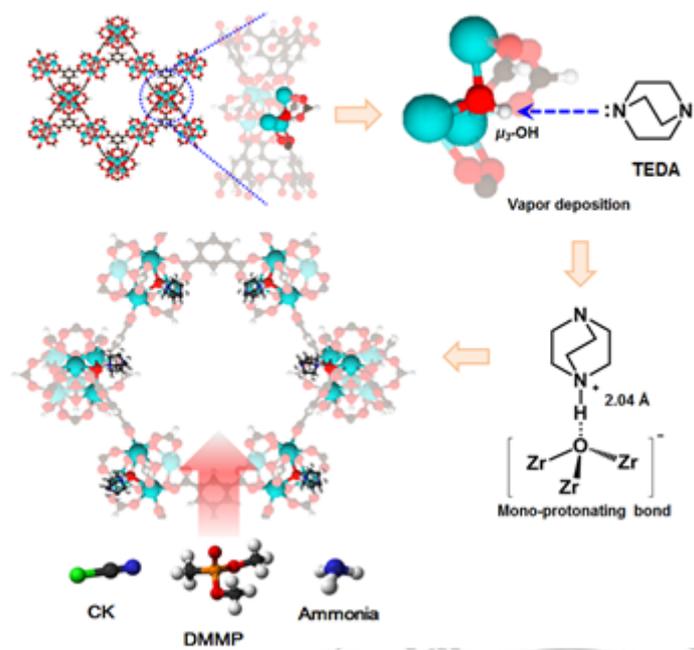
Direct Functionalization of Metal-Organic Framework Node: Targeting Diamine Deposition for Removing Toxic Chemicals in Humid Environment

Ga-Young Cha, Young Kyu Hwang*

Korea Research Institute of Chemical Technology, Korea

Zirconium-based metal-organic frameworks (Zr-MOF) have been extensively investigated to efficiently remove chemical warfare agents and simulant as well as industrial toxic gas due to their chemical and thermal stability. Herein, we have developed a selective functionalization of Zr-bridging hydroxo species on Zr-nodes of MOFs with a triethylenediamine (TEDA) through gas phase acid-base reaction, successfully leading to formation of ionic frameworks. Remarkably, TEDA-MOF-808 show outstanding performance for removal of toxic chemicals, such as CK, DMMP and ammonia in humid conditions. In situ analyses demonstrate how the TEDA is selectively deposited on Zr-bridging hydroxo sites (μ_3 -OH) and also operando FT-IR spectra show why TEDA grafted MOF-808 has superior sorption characteristics. This work highlights the advantages of diamine-grafted MOFs for the preparation of versatile adsorbents, extending their scope to catalytic applications.

MOF-808



Poster Presentation : **INOR.P-194**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

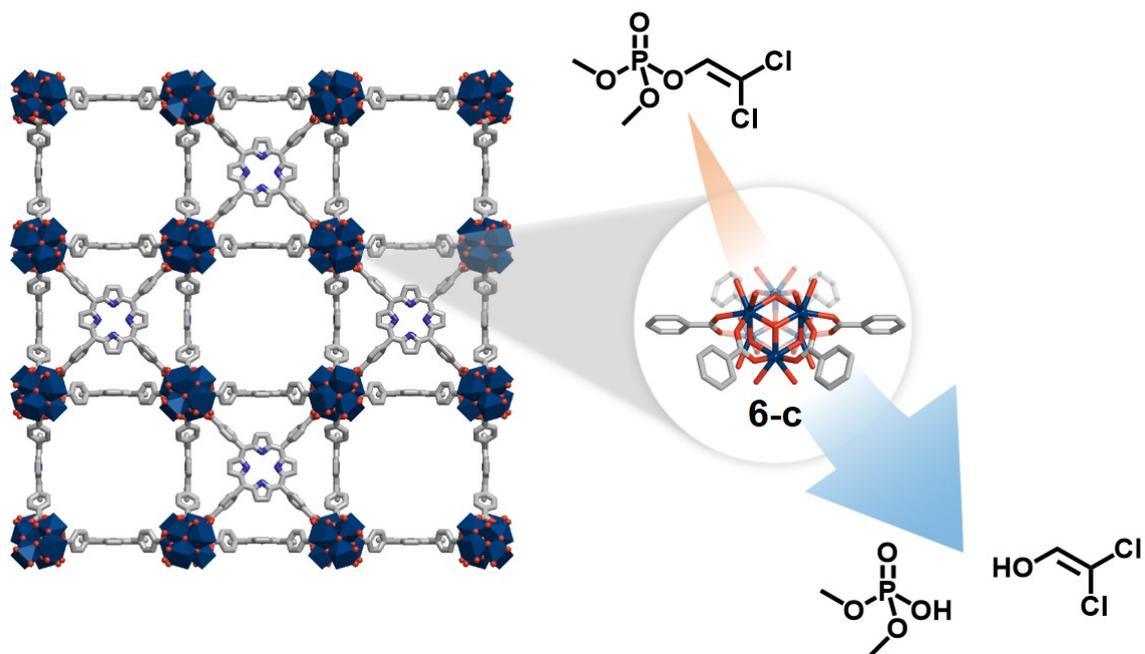
Metal-Organic Frameworks for Catalytic Detoxification of Pesticides

**Dongsik Nam, Yeongjin Kim, Miyeon Kim¹, Joochan Nam, Seonghun Kim, Eunji Jin,
Chang Yeon Lee¹, Wonyoung Choe^{*}**

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

¹*Department of Energy and Chemical Engineering, Incheon National University, Korea*

Pesticides are chemicals widely used for agricultural industry, despite their negative impact on health and environment. Although various methods have been developed for pesticide degradation to remedy such adverse effects, conventional materials often take hours to days for complete decomposition and are difficult to recycle. Here, we present rapid degradation of organophosphate pesticides with a Zr-based metal-organic framework (MOF), showing complete degradation within 15 minutes. MOFs with different active site structures (Zr node connectivity and geometry) were compared, and a porphyrin-based MOF with 6-connected Zr nodes showed remarkable degradation efficiency with half-lives of a few minutes. Such high efficiency was further confirmed in a simple flow system for several cycles. This study reveals that MOFs can be highly potent heterogeneous catalysts for organophosphate pesticide degradation, suggesting that coordination geometry of Zr node significantly influences the catalytic activity.



Poster Presentation : **INOR.P-195**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Comparative Investigations into Anticancer Activity of Copper Bis(Thiosemicarbazone) and Bis(Semicarbazone) Complexes

Hanae Lim, Hyeri Jeon, Yool Lee, Seungwoo Hong*

Department of Chemistry, Sookmyung Women's University, Korea

Extensive investigations on the anticancer activity of thiosemicarbazone, semicarbazone, and their derivatives have been triggered to their development of practical application *in vitro* and *in vivo* up to date. As copper is either vital nutrient and potentially dangerous cytotoxin in the biological system, there has been great attention on the pharmaceutical and medicinal properties of copper complexes, especially for treatment of cancer. In this context, we synthesized four structurally different copper complexes bearing thiosemicarbazone and semicarbazone and characterized them by using various spectroscopic methods including X-ray crystallography. The anti-proliferative activity of these copper complexes were evaluated by measuring the concentration of reactive oxygen species (ROS) generated in the presence of ascorbic acid and the level of cleaved DNA *in vitro*. Among abovementioned copper complexes, copper complexes bearing bis(semicarbazone) and bis(semicarbazone-benzyl) showed superior production of ROS species and enhanced level of cleaved DNA upon 24 h incubation. Of note, interest in semicarbazone type ligand bearing copper complexes has centered on their anti-cancer potency due to both the redox activity leading to ROS formation and DNA binding activity. Upon incubation of these four copper complexes with HCT116 cells, copper bis(semicarbazone-benzyl) complex effectively resulted in the cell death while other complexes are more an less lethal. Through ROS assay, Western blot analysis of cleaved DNA, and immunocytochemistry, the structure-anticancer activity relationship in combination with their electrochemical properties was established and further provided synthetic strategies of bis(semicarbazone) type anticancer agents.

Poster Presentation : **INOR.P-196**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

An end-on bis(μ -hydroxo) dimanganese(II,III) azide complex for C–H bond and O–H bond activation reactions

Hyeri Jeon, Hanae Lim, Yool Lee, Seungwoo Hong*

Department of Chemistry, Sookmyung Women's University, Korea

There is an increasing interest in the reactivity studies of Mn-hydroxo intermediates in the C–H bond activation and O–H bond activation reactions. We report the synthesis of an end-on dinuclear manganese(II) azide complex with two bridging azide ligands that served as a precursor for the formation of an end-on bis(μ -hydroxo) dinuclear manganese(II,III) azide complex upon oxidation by organic peroxide or peracids. In C–H bond and O–H bond activation reactions, the end-on bis(μ -hydroxo) dinuclear manganese(II,III) azide complex exhibits moderate reactivity with substrates having weak C–H bond and O–H bond dissociation energy via H-atom abstraction reaction in a concerted manner. The reaction pathway was interpreted by density functional theory calculations, suggesting that the dissociation of the end-on bis(μ -hydroxo) dinuclear manganese(II,III) azide complex resulting in the formation of a mononuclear manganese(III)-hydroxo and a manganese(II)-hydroxo complexes occurred prior to the H-atom abstraction and the former complex is capable of conducting the oxidation reactions of substrates.

Poster Presentation : **INOR.P-197**

Inorganic Chemistry

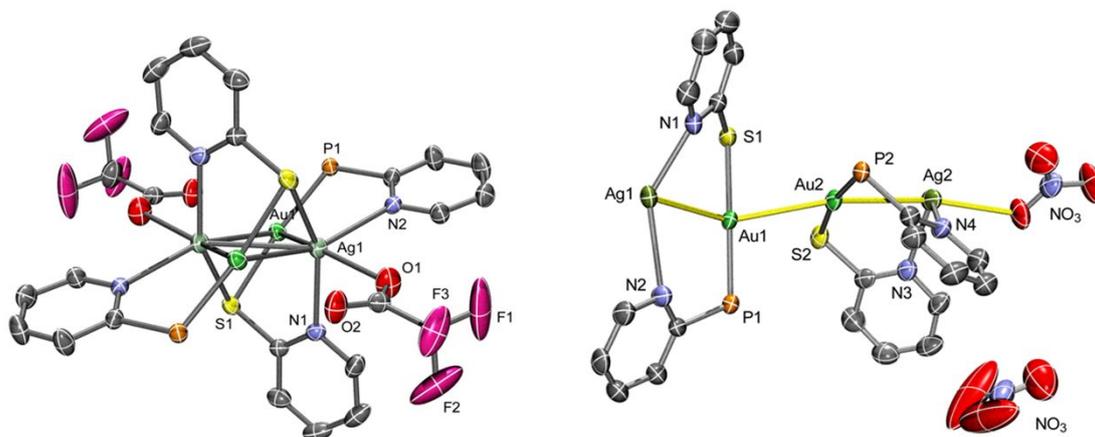
Zoom 5 FRI 15:00~16:00

Anion effects of M-M interaction in Au(I)-Ag(I) Complexes

Jiyeong Song, Young-A Lee*

Department of Chemistry, Jeonbuk National University, Korea

A new series of Au(I)-Ag(I) heterometallic complexes, $[\text{AuAg}(\text{Spy})(\text{PPh}_2\text{py})]\text{X}$ ($\text{X} = \text{BF}_4^-, \text{PF}_6^-, \text{ClO}_4^-, \text{CF}_3\text{CO}_2^-, \text{CF}_3\text{SO}_3^-, \text{NO}_3^-$), have been synthesized, and their physical properties and luminescence were studied in the solid state at room temperature and at 77 K. According to the change of anion, we were expected to control of metal-metal interaction. It will show us competition of d^{10} metals like Au(I)-Au(I), Au(I)-Ag(I), Ag(I)-Ag(I). X-ray characterizations on the single crystals have provided the dimeric ($\text{X} = \text{CF}_3\text{CO}_2^-, \text{CF}_3\text{SO}_3^-$) or polymeric form ($\text{X} = \text{NO}_3^-$) of $[\text{AuAg}(\text{Spy})(\text{PPh}_2\text{py})]\text{X}$ depending on the anion types. For the complexes with $\text{X} = \text{CF}_3\text{CO}_2^-, \text{CF}_3\text{SO}_3^-$, the two of $[\text{AuAg}(\text{Spy})(\text{PPh}_2\text{py})]$ moiety are bound via the transannular Au-Au interaction (5.050 Å), Ag-Ag interaction (3.03 – 3.07 Å) and bridging sulfur (Ag(1)-S(1), 2.50 – 2.54 Å; Au(1)-S(1), 2.33 Å). Despite of the similar skeletal structure, complexes with $\text{X} = \text{NO}_3^-$ shows the infinite chains through the additional Au...Au interactions (2.8862(2) Å) and anion binding effects. These materials are luminescent in the solid state and exhibits an emission band at 470nm ($\lambda_{\text{ex}} = 360\text{nm}$) at 77K.



Poster Presentation : **INOR.P-198**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Antibacterial Effects and in-vitro Cytotoxicity for Cu-MOF Imbedded Polysiloxane (PS@Cu-MOF)

So-Hyeon Yang, Youngmee Kim¹, Sung-Jin Kim², Do Nam Lee^{3,*}

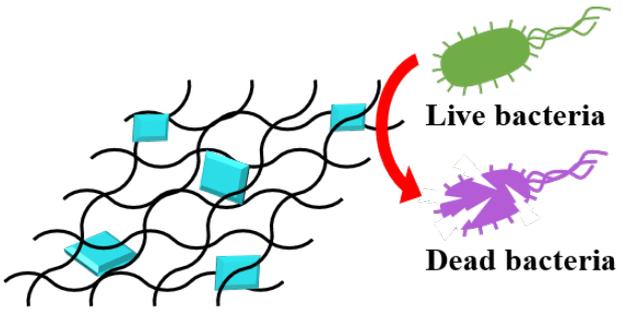
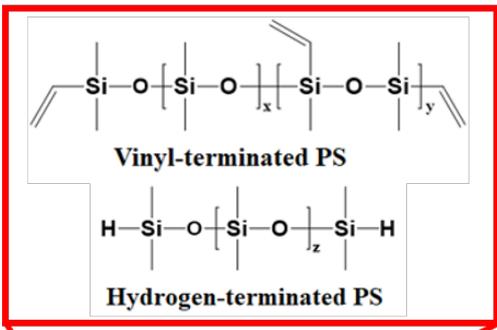
Department of Chemistry and Nanoscience, Ewha Womans University, Korea

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

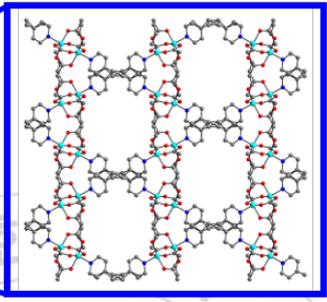
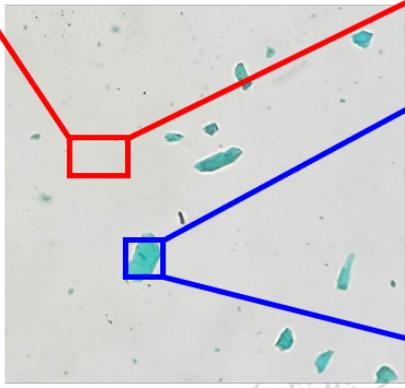
²*Department of Chemistry, Ewha Womans University, Korea*

³*Ingenium College of Liberal arts, Kwangwoon University, Korea*

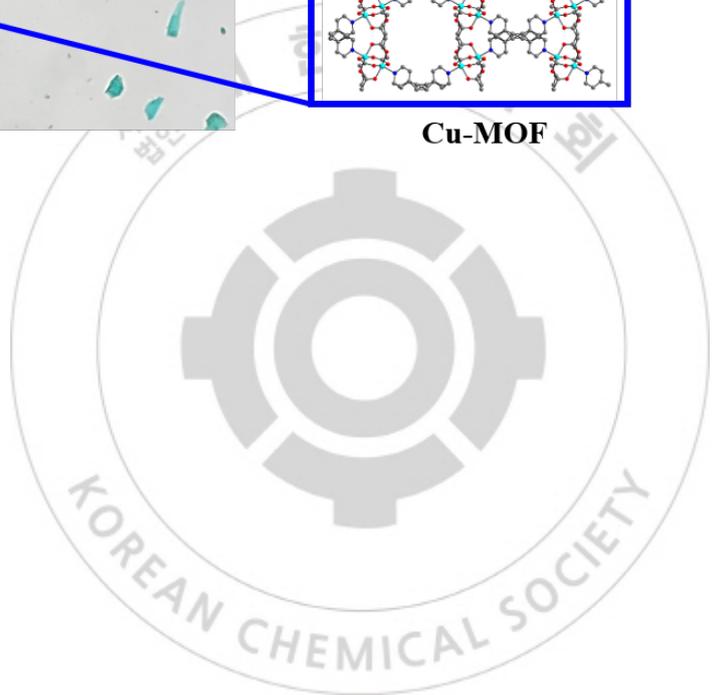
Polysiloxanes (PSs) have been widely used as lubricants, varnishes, paints, release agents, adhesives, and insulators in the industry, and their applications have been expanded to include the development of new biomedical materials. The surface of PS was modified with Cu-MOF via a hydrosilylation reaction of vinyl-terminated and H-terminated PSs at 25 °C. The Cu-MOF-embedded PS (PS@Cu-MOF) exhibited superior antibacterial properties toward the tested bacteria (E. coli, S. aureus, and MRSA) than the control PS at a concentration of 100 µg·mL⁻¹, and it showed a low cytotoxicity toward mouse embryonic fibroblasts at the same concentration. Release tests of the Cu(II) ion showed PS@Cu-MOF to be particularly stable in a phosphate-buffered saline(PBS) solution. The low cytotoxicity and bactericidal activities of PS@Cu-MOF render it a promising candidate for use in medicinal applications, such as in implants, skin-disease treatment, wound healing, and drug delivery.



Cu-MOF embedded PS



Cu-MOF



Poster Presentation : **INOR.P-199**

Inorganic Chemistry

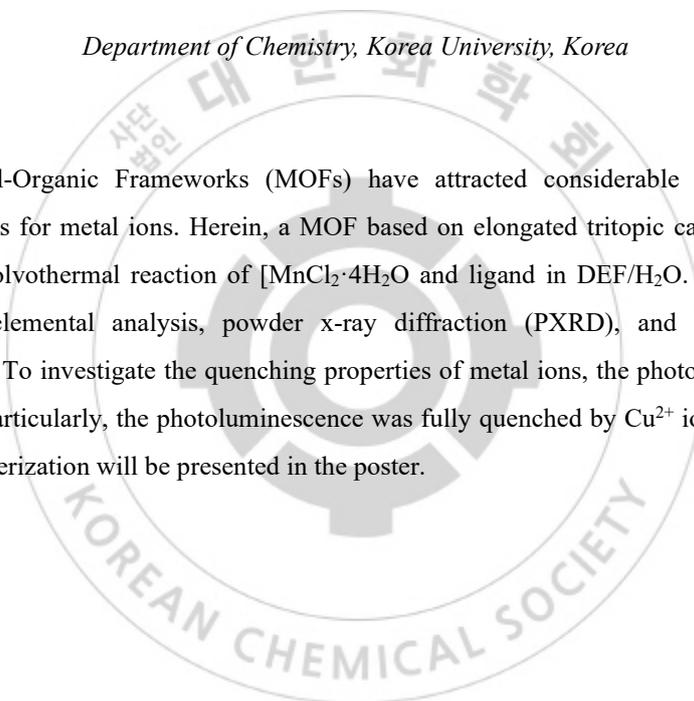
Zoom 5 FRI 15:00~16:00

Photoluminescence Quenching of a Mn(II)-Based Metal-Organic Framework toward Cu²⁺ ion

Hyojin Kim, Minjung Kang, Jong Hyeak Choe, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Luminescent Metal-Organic Frameworks (MOFs) have attracted considerable interest in terms of fluorescence sensors for metal ions. Herein, a MOF based on elongated tritopic carboxylate ligand was synthesized by a solvothermal reaction of [MnCl₂·4H₂O and ligand in DEF/H₂O. Mn-based MOF was characterized by elemental analysis, powder x-ray diffraction (PXRD), and differential scanning calorimetry (DSC). To investigate the quenching properties of metal ions, the photoluminescence studies were carried out. Particularly, the photoluminescence was fully quenched by Cu²⁺ ion. Detailed synthetic scheme and characterization will be presented in the poster.



Poster Presentation : **INOR.P-200**

Inorganic Chemistry

Zoom 5 FRI 15:00~16:00

Selective adsorption of ethane over ethylene in nickel-based metal-organic frameworks

Minjung Kang, Jong Hyeak Choe, Hyojin Kim, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Ethylene is one of the most valuable chemicals for industrial polymer production. The effluent of the steam cracking process contains 5%-10% ethane that must be separated to produce the high-purity ethylene for the polymerization reaction. We synthesized Ni-based MOFs and evaluated its ethane selectivity for ethylene purification. The Ni-based MOFs showed high adsorption amount at low pressure based on the single component isotherms of ethane and ethylene, and exhibit selective uptake of ethane over ethylene. 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 presented in the poster.

Poster Presentation : **INOR.P-201**

Inorganic Chemistry

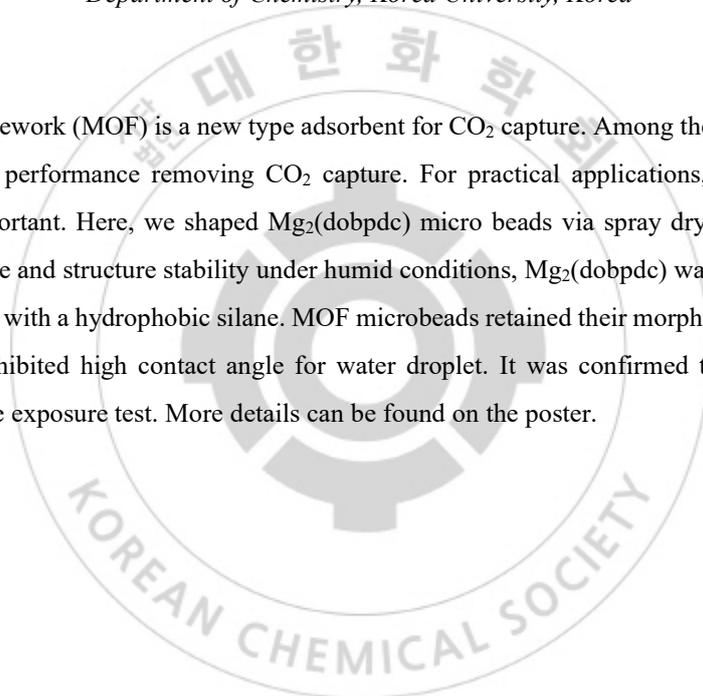
Zoom 5 FRI 15:00~16:00

MOF-based micro-beads with silane coating for CO₂ capture

Jong Hyeak Choe, Hyojin Kim, Minjung Kang, Chang Seop Hong*

Department of Chemistry, Korea University, Korea

Metal-organic framework (MOF) is a new type adsorbent for CO₂ capture. Among the MOFs, M₂(dobpdc) shows outstanding performance removing CO₂ capture. For practical applications, suitable shaping of M₂(dobpdc) is important. Here, we shaped Mg₂(dobpdc) micro beads via spray dry method. In order to improve CO₂ uptake and structure stability under humid conditions, Mg₂(dobpdc) was functionalized with diamine and coated with a hydrophobic silane. MOF microbeads retained their morphology, enhanced CO₂ adsorption, and exhibited high contact angle for water droplet. It was confirmed that crystallinity was maintained after the exposure test. More details can be found on the poster.



Poster Presentation : **INOR.P-202**

Inorganic Chemistry

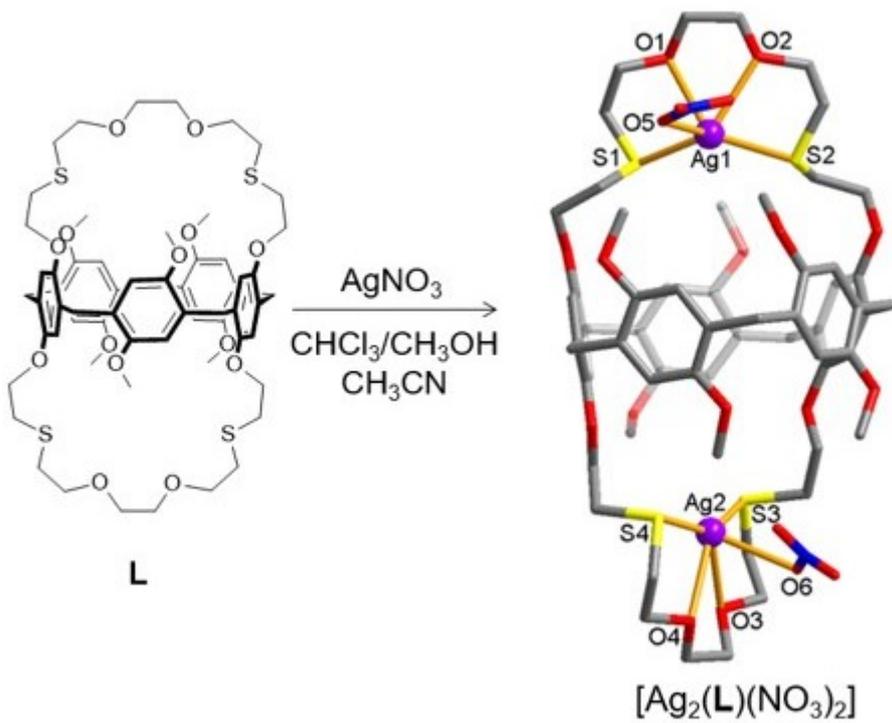
Zoom 5 FRI 15:00~16:00

Pillar[5]-*bis*-thiacrown: Synthesis and Characterization of Silver(I) Complexes with Organic Guest

Yelim Lee, Eunji Lee*

Department of Chemistry , Gangneung-Wonju National University, Korea

The pillar[5]-*bis*-thiacrown (**L**) and its silver(I) complexes with organic guests were synthesized and structurally characterized. **L** was synthesized from ring closure reaction between corresponding pillar[5]arene-dibromide and 3,6-dioxa-1,8-octanedithiol in the presence of K_2CO_3 . Reaction of **L** with $AgNO_3$ afforded disilver(I) complex of formula $[Ag_2L(NO_3)_2]$, with an $Ag \cdots Ag$ separation of 11.3 Å. Furthermore, the silver(I) nitrate complex forms a disilver(I) metallocage with 1,2-dicyanoalkane (**C2**), in which **C2** molecule exists inside the pillar[5]arene cavity. The complexation studies of **L** with organic guests both in solution and solid states are in progress.



Poster Presentation : **INOR.P-203**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Triple C–F Bond Activation of Fluoroarenes by N-heterocyclic Carbenes Generating Trisubstituted N-Heterocyclic Imidazoliums

Seoung Su Kim, Eunsung Lee^{1,*}

Pohang university of Science and TECHnology, Korea

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

N-heterocyclic carbenes (NHCs) has been studied in depth focusing on their unique ability not only to support transition metal complexes in a range of valuable catalytic applications, but also to activate small molecules directly, and to stabilize various reactive species. In particular, free NHCs are now well-known to activate such chemical bonds as C–H, H–H and N–H, which had traditionally been the domain of reactivity of transition metal complexes. We have been exploring activation of C–F bonds utilizing NHCs for various applications such as catalysis and material science. For example, IPr, one of well-known NHCs, reacts with octafluorotoluene by an unexpected sequential substitution of fluorides in two separate rings to afford tetrasubstituted imidazolium salt, followed by the formation of Ag(I) and Au(I) complexes as a new entity of a novel abnormal NHC ligand. As a better and challenging extension, here we report triple C–F bond activation of fluoroarenes by N-heterocyclic carbenes 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-204**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

A Molecular Based Chromophore-Catalyst Electroassembly for Photoelectrochemical Water Oxidation

So-Yeon Kim, Kyung-Ryang Wee*

Department of Applied Chemistry, Daegu University, Korea

We describe an electrochemically polymerization procedure for preparing chromophore-catalyst assemblies on the nanoparticle metal oxide electrode surfaces for the long-term stable photoelectrochemical water oxidation in various aqueous conditions. With water as the solvent, a troublesome arises from loss of surfacebound chromophores and catalysts due to desorption and decomposition from the metal oxide surface. Therefore, the thiophene derivative is coated deeply on the metal oxide electrode to stabilize the surface, and the chromophore-catalyst assembly for water oxidation is assembled on top of it by reductive electropolymerization. Also, the electropolymerization strategy is a simple toolkit that provides synthetic control and well-defined structures. Based on earlier procedures for preparing cross-linked electropolymerized films by reductive coupling of vinyl derivatized polypyridyl complexes, electroassembly offers the advantage of on-surface synthesis without prior covalent bond formation. On the nanoparticle metal oxide films as a photoanode, excitation of the assembly with 1 sun (100 mW cm^{-2}) illumination in phosphate buffer with an applied bias leads to water splitting in a dye-sensitized photoelectrosynthesis cell (DSPEC) with a Pt cathode. Over multiple hour photolysis experiment, electrochemically prepared photoanode shows sustained water splitting with no significant photocurrent decrease. Instability of the surface bound chromophore in its oxidized state in the phosphate buffer leads to a gradual decrease in photocurrent and to the relatively modest faradaic efficiencies. These results indicate that the chromophore-catalyst electroassembly coated with thiophene derivative is a simple toolkit to make stable DSPEC system for solar fuel production.

Poster Presentation : **INOR.P-205**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Iron-catalyzed Defluoroborylation of Aryl Fluorides

Soocheon Kim, Eunsung Lee*

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

Fluorine atoms play a key role in a range of unique physical and chemical properties in such widely used fluorinated molecules as pharmaceuticals, agrochemicals, and materials. Utilities in these applications have made significant synthetic developments over the past decades to manage the manipulation of C–F bonds. In particular, a variety of methods to generate aromatic C–F bonds now offer quick access to desired and complex fluorinated molecules, and thus late-stage ^{18}F -fluorination reactions are being developed to expand the scope of positron emission tomography (PET) tracers. With these synthetic tools, aryl fluorides have become more ubiquitous, and now functionalization of inert C–F bonds offers new synthetic opportunities. Therefore, borylation of such inert C–F bond is our particular interest as arylboronic esters are a versatile functional group that enables further transformation. In particular, combined with the late-stage ^{18}F fluorination reaction of arylboronic esters, C–F bond borylation would enable the straightforward conversion of readily available fluorinated pharmaceuticals into ^{18}F -labeled PET tracers. Herein, an iron-catalyzed defluoroborylation of aryl fluorides is described. This reaction can be operated from the commercial iron salts and inexpensive ligand with high selectivity of C–F bonds over C–H bonds. The details will be discussed.

Poster Presentation : **INOR.P-206**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Tris(5-phenyl-1*H*-1,2,4-triazolyl)iridium(III) Complex and Its Excellent Performance in Blue Phosphorescent Organic Light-Emitting Diodes

Chan Hee Ryu, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Herein, we prepared a phenyl-1,2,4-triazole-based *facial*-homoleptic iridium(III) complex, **TzIr** (fac-tris(1-(2,6-diisopropylphenyl)-3-methyl-5-phenyl-1*H*-1,2,4 triazolyl) iridium(III)). The complex was fully characterized by multinuclear NMR spectroscopy and elemental analysis. The molecular structure was definitively determined by single-crystal X-ray diffraction. The complex shows a definite blue-emission band ($\lambda_{em} = 456$ nm) in the solution and film states at ambient temperature. Moreover, this complex exhibits considerably high phosphorescent quantum efficiency (80%) and thermal stability ($T_{d5} = 362$ °C). Multilayer phosphorescent OLEDs using **TzIr** as the emitter and 3,3-di(9*H*-carbazol-9-yl)biphenyl (mCBP)/ 9-(3'-(9*H*-carbazol-9-yl)-5-cyano-[1,1'-biphenyl]-3-yl)-9*H*-carbazole-3-carbonitrile (CNmCBPCN) as the mixed host are fabricated. The devices exhibit outstanding performance, with a high external quantum efficiency (27.8%), current efficiency (38.7 cd A⁻¹), and CIE_y (y coordinate value of the Commission Internationale de l'Éclairage color space) less than 0.18. The results of this study indicate that this novel 1,2,4-triazole-based dopant, **TzIr**, is a promising candidate for developing highly efficient blue-phosphorescent emitters for use in OLEDs.

Poster Presentation : **INOR.P-207**

Inorganic Chemistry

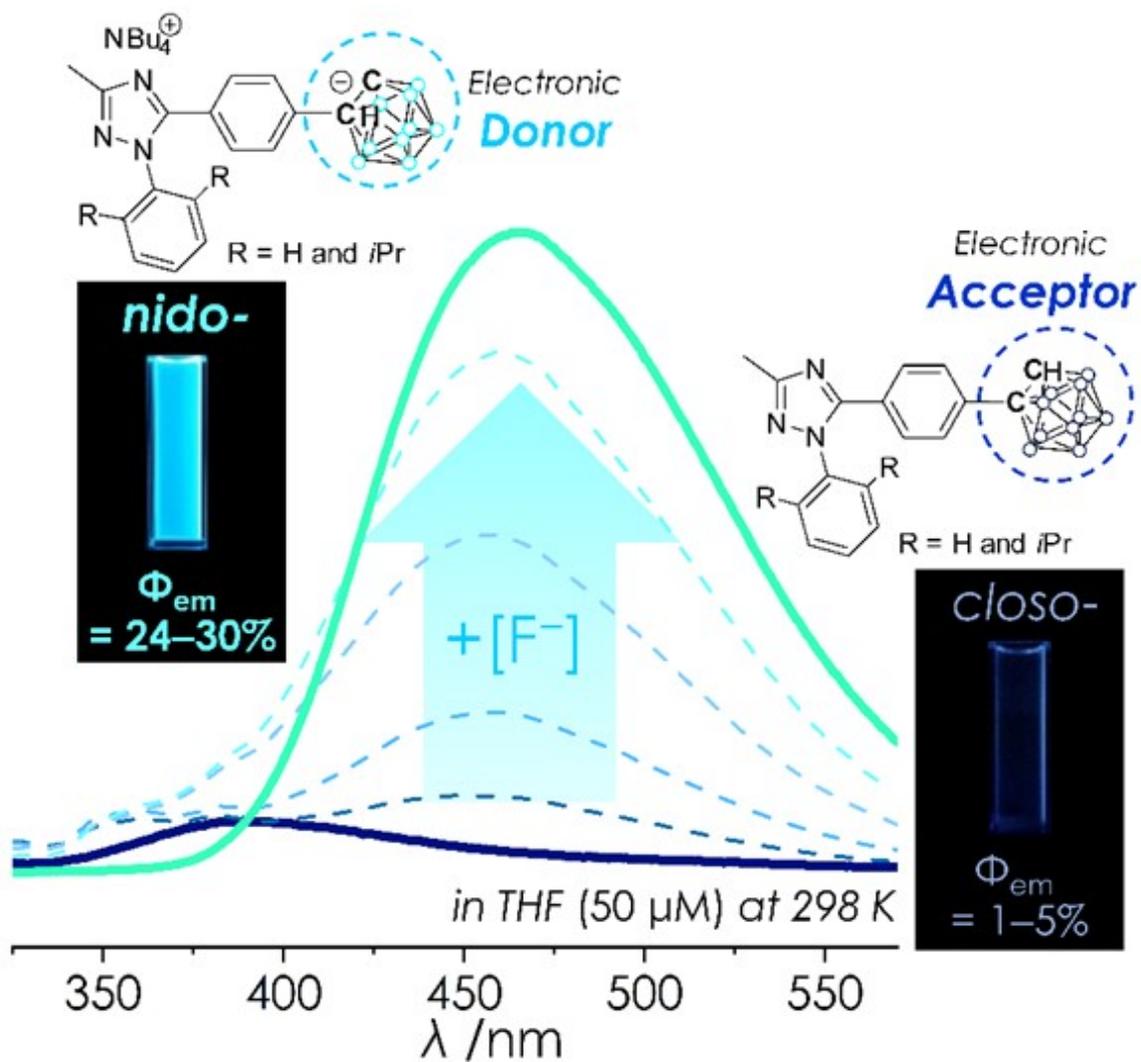
Zoom 5 FRI 16:00~17:00

Intriguing Photophysical Properties Changed by Deboronation of Triazole-appended *Closo-o*-carboanyl Luminophores

Mingi Kim, Sehee Im, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

Triazole-appended *closo*- (**CB1** and **CB2**) and *nido-o*-carboranyl (*nido*-**CB1** and *nido*-**CB2**) compounds were prepared and fully characterized using multinuclear NMR spectroscopy and elemental analysis. In addition, the solid-state molecular structures for both *closo*-compounds were confirmed by X-ray crystallography. The *closo-o*-carboranyl compounds exhibited dual emissive patterns in the rigid state (in THF at 77 K), which were assignable to a π - π^* local excitation (LE)-based emission on the triazole moieties at *ca.* 380 nm, and to an intramolecular charge transfer (ICT)-based emission at *ca.* 460 nm in which the *closo-o*-carborane units acted as the acceptor (A), at 298 K in THF, the LE-based emission dominated. In contrast, the *nido*-compounds revealed an intense ICT-based emission in which the *nido-o*-carborane units reversibly acted as the donor (D). In particular, the positive solvatochromic effects of both *nido*-compounds and the results of the theoretical calculations supported the electronic role of the *o*-carboranyl unit in each compound. Interestingly, a comparison of the radiative (k_r) and nonradiative (k_{nr}) decay constants between the *closo*- and *nido*-compounds, which were calculated using the measured quantum efficiencies (Φ_{em}) and decay lifetimes (τ_{obs}), suggested that the ICT-based radiative decay of *nido*-compounds occurred more efficiently than the LE-based decay of *closo*-compounds. These results implied that the emission from the *closo*-compounds was dramatically enhanced by the deboronation reaction upon exposure to an increasing concentration of fluoride anions, and finally became the emission color of the *nido*-compounds.



Poster Presentation : **INOR.P-208**

Inorganic Chemistry

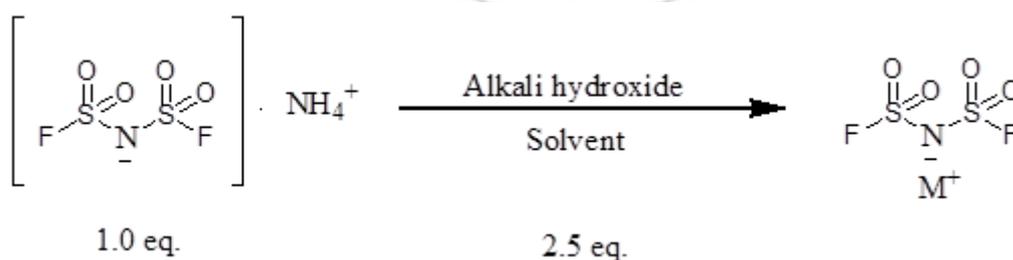
Zoom 5 FRI 16:00~17:00

Facile method for preparing lithium bis(fluorosulfonyl)imide [LiFSI]

Seok Ju Lee, Mingi Chu, Dong wook Kang*

Department of Pharmaceutical Engineering, Daegu Catholic University, Korea

Lithium bis(fluorosulfonyl)imide [LiFSI] is a useful compound used in various fields such as an electrolyte, ion conductive material or anion of an ionic liquid, electrolyte additive for a fuel cell, and selective absorber material. LiFSI salt can be prepared by carrying out a cation exchange reaction with lithium hydroxide to a bis(fluorosulfonyl)imide [FSI] ammonium salt. In this case, butyl acetate (B.A.) is used as the optimum solvent for the reaction. However, since B.A. has a higher boiling point than other organic solvents, it takes a considerable amount of time to remove it, thereby resulting in a high manufacturing cost. In this study, LiFSI is efficiently prepared using various organic solvent conditions. Isobutyl acetate (I.A.) and ethyl propionate (E.P.) with relatively low boiling points were used as solvents instead of B.A. Results obtained herein suggest that less time was required for the solvent removal process, and the likelihood of the solvent remaining in the final product was low, thereby resulting in excellent purity. In addition, under the co-solvent condition of I.A.:E.P. = 1:4, we obtained LiFSI in the highest yield in a short period of time.



Poster Presentation : **INOR.P-209**

Inorganic Chemistry

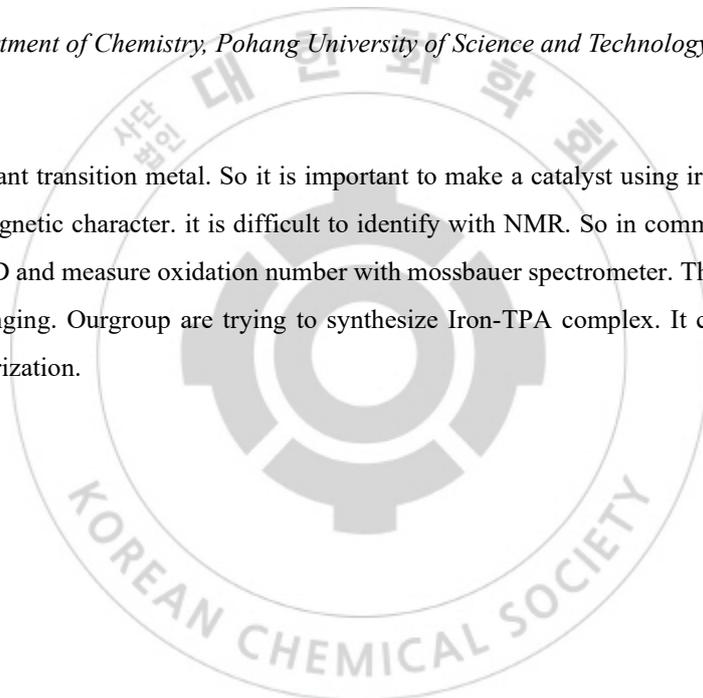
Zoom 5 FRI 16:00~17:00

New Iron Complexes Supported by Tris(4,6-di-tert-butyl-2-hydroxybenzyl-Amine)

Gunhee Lee, Eunsung Lee*

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

Iron is earth abundant transition metal. So it is important to make a catalyst using iron. but iron complex usually has paramagnetic character. it is difficult to identify with NMR. So in common, their structure is identified with XRD and measure oxidation number with mossbauer spectrometer. Therefore, iron catalyst synthesis is challenging. Ourgroup are trying to synthesize Iron-TPA complex. It can be used coupling reaction or polymerization.



Poster Presentation : **INOR.P-210**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Electrocatalytic Reduction of CO₂ by Polypyridyl Co Complexes

Wonjung Lee, Seungjin Song¹, Junhyeok Seo^{*}

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

¹Chemistry, Gwangju Institute of Science and Technology, Korea

Climate crisis increases research interests in CO₂ fixation/recycling methods. Electrocatalytic CO₂ reduction is a simple pathway for CO₂ transformation, but the poor selectivity and efficiency remain challenges because of a competitive reaction (proton reduction) and various CO₂ reduction products such as CO, HCO₂H, etc. For the goal, researchers have developed transition metal complexes using earth-abundant metals, and polypyridyl complexes have obtained research interests due to the promising electrocatalytic activity. We study the CO₂ reduction reactivity of pincer-type complexes and polypyridyl complexes, and recently, several Co-polypyridyl complexes have shown interesting CO₂ reduction activity. In this poster, I will show the CO₂ reactivity of Co polypyridyl complexes and the utilization of pincer-type ligands.

Poster Presentation : **INOR.P-211**

Inorganic Chemistry

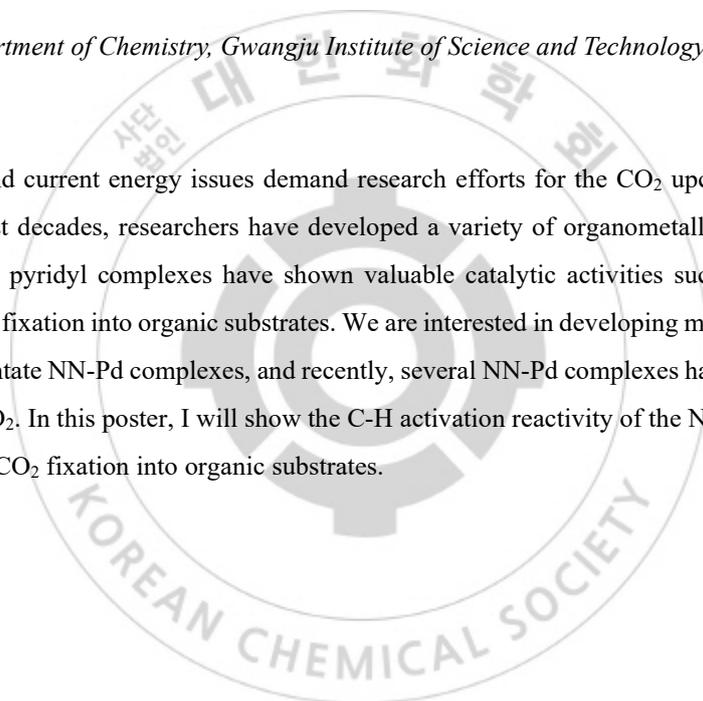
Zoom 5 FRI 16:00~17:00

CO₂ Reactivity of NN-Pd Complexes and Application to CO₂ Fixation into Organic Substrates

JuEun Lee, Junhyeok Seo*

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

Global warming and current energy issues demand research efforts for the CO₂ upcycling to high-value products. In the last decades, researchers have developed a variety of organometallic complexes for the CO₂ reactions, and pyridyl complexes have shown valuable catalytic activities such as CO₂ reduction, hydrogenation, and fixation into organic substrates. We are interested in developing methodologies for CO₂ fixation using bidentate NN-Pd complexes, and recently, several NN-Pd complexes have shown interesting reactivities with CO₂. In this poster, I will show the C-H activation reactivity of the NN-Pd complexes and the applications to CO₂ fixation into organic substrates.



Poster Presentation : **INOR.P-212**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Experiments for the Better Determination of Beta-Particles

Hye-Sung Jung, Chung Hun Han¹, Hee-Jung Im^{2,*}

department of chemistry & cosmetics, Jeju National University, Korea

¹*Jeju National University, Korea*

²*Department of Chemistry, Jeju National University, Korea*

Strontium-90 emits a beta-particle and decays into yttrium-90. At this time, the beta-particles released affect a human body, and liquid scintillation counting (LSC) is used to detect such beta-particles. A so-called cocktail method that mixes samples and liquid scintillators is used in conventional LSCs. In the cocktail method, the degree of miscibility or solubility between samples and scintillators, and depositional phenomena reduce the reproducibility of the experiment. Therefore, in this experiment, the method of measuring beta-particles after separating samples and scintillators each other is presented. In addition, several experiments are conducted to investigate the efficiency and tendency of the new method using a quenching curve.

Poster Presentation : **INOR.P-213**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Adsorption Mechanism between Ag Nanoparticles or Ag⁺ Ion Included in Mercaptopropyl Functionalized Silica Gels and Gaseous CH₃I

Jeong Woo Hong, Hee-Jung Im*

Department of Chemistry, Jeju National University, Korea

To include silver in silica gels functionalized with mercaptopropyl, silica gels were placed in a 2-propanol in which AgNO₃ was dissolved. After then, the silica gels in the solution were irradiated with an electron beam to produce Ag nanoparticle-embedded mercaptopropyl silica gels or left unattended to Ag⁺ ion-coated mercaptopropyl silica gels. After all, six types of silica gels differentiated by the oxidation states of silver and the existence of a functionalized mercaptopropyl ligand were prepared. The purpose of this study is to investigate the adsorption mechanism and interaction tendency between prepared silica gels and gaseous methyl iodide for each silver state through various spectroscopic analyses. In addition, the cleavage of the functionalized mercaptopropyl during the electron-beam irradiation and differences in the interaction between mercaptopropyl and silver according to the silver states are also discussed.

Poster Presentation : **INOR.P-214**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Electrochemical H₂ Evolution by Pincer-type NNN-Co Complexes

Seungjin Song, Junhyeok Seo^{1,*}

Chemistry, Gwangju Institute of Science and Technology, Korea

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

Dihydrogen is a carbon-free and renewable energy carrier, and the electrochemical H₂ evolution reaction (HER) is spotlighted as a sustainable energy cycling method. Pt is the best electrocatalyst, but researchers develop electrode materials and transition metal complexes using earth-abundant metals. We try to develop H₂ catalysts with pincer-type ligand-coordinated Co complexes. Pincer-type ligand has been widely used in organometallic catalysis because it well stabilizes a central metal ion during catalytic reactions. Furthermore, the electronic connectivity with transition metals expands the utilization of pincer complexes as electrocatalysts. In the synthetic aspect, the pincer-type ligand structure can provide platforms to attach functional groups. We enhanced H₂ evolution efficiency using pincer-type NNN-Co complexes assisted by a proton-relay agent in the secondary coordination sphere. In this poster, I will show the hydrogen reactivity of NNN-Co complexes with electrochemical data, and discuss current understandings of the reaction mechanisms with DFT calculation results.

Poster Presentation : **INOR.P-215**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

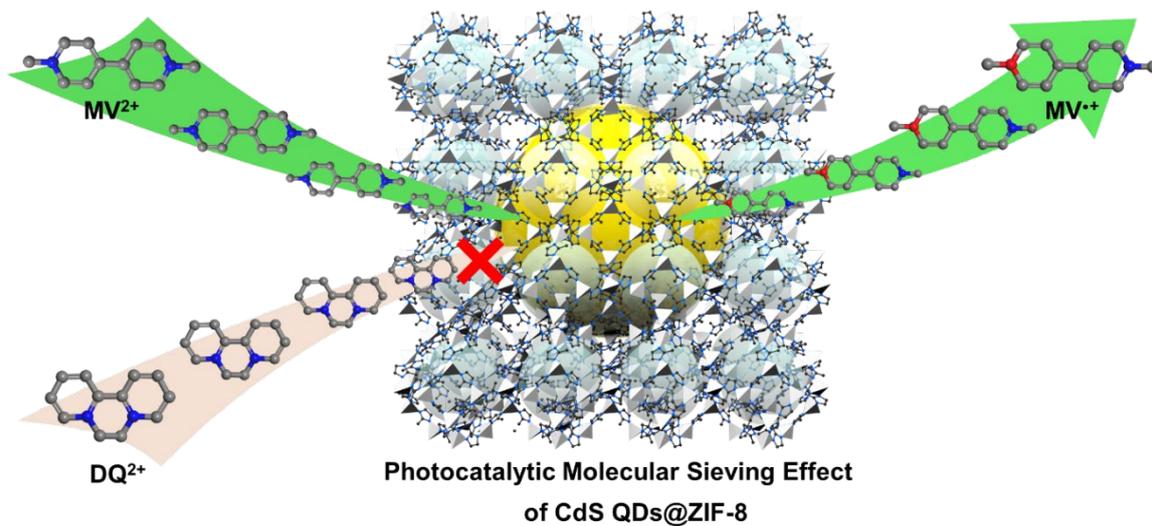
Strategy for Encapsulation of CdS Quantum Dots into Zeolitic Imidazole Frameworks for Photocatalytic Activity

Hyun Sung Kim^{*}, Yerim Son¹

Department of Chemistry, Pukyong National University, Korea

¹*Chemistry, Pukyong National University, Korea*

Encapsulating CdS quantum dots (QDs) into zeolitic imidazole framework-8 (ZIF-8) can offer several advantages for photocatalysis. Various types of capping agents have been used to encapsulate QDs into ZIF-8 nanopores. An effective method for encapsulating CdS QDs into ZIF-8 is to use 2-mercaptoimidazole as the capping agent. This is because 2-mercaptoimidazole is similar to the imidazolate ligands of ZIFs and can be used for capping active species with simultaneous encapsulation during the crystal growth of ZIF-8. Compared to other widely used capping agents such as polyvinylpyrrolidone (PVP), using 2-mercaptoimidazole for encapsulating CdS QDs into ZIF-8 revealed photocatalytic effects along with the molecular sieving effect when using differently sized molecular redox mediators such as methyl viologen (MV²⁺) and diquat (DQ²⁺).



Poster Presentation : **INOR.P-216**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Iron-catalyzed Demethoxyborylation of Aryl Methoxides

Eunsung Lee^{*}, Jongheon Jeong

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

$C(sp^2)$ -O electrophiles have been regarded as reliable alternatives to aryl halides as coupling partners in the cross-coupling reactions due to the absence of toxic halogenated byproducts, inertness, low price, and ready availability. Recently, a series of transition metal-catalyzed cross-coupling reactions utilizing relatively active C-O electrophiles such as aryl sulfonates, phosphates, esters, or carbamates were 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, the methoxy group can be utilized as an ortho C-H bond functionalization director in late-stage functionalization. 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 operated from the commercial iron salts and inexpensive simple ligand with 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 bond into diverse chemical bonds.

Poster Presentation : **INOR.P-217**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

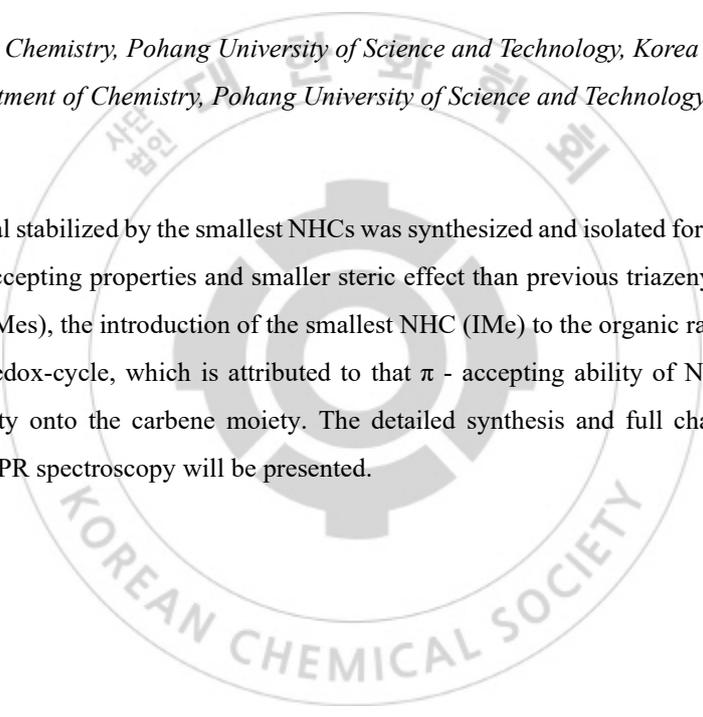
Synthesis and Reactivity of N-Heterocyclic Carbene-Based Sterically Less Hindered Triazenyl Radical

Jaelim Kim, Eunsung Lee^{1,*}

Chemistry, Pohang University of Science and Technology, Korea

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

New triazenyl radical stabilized by the smallest NHCs was synthesized and isolated for full characterization. Despite weaker π -accepting properties and smaller steric effect than previous triazenyl radicals stabilized by NHCs (IPr and IMes), the introduction of the smallest NHC (IMe) to the organic radicals could support to obtain 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 radicals including EPR spectroscopy will be presented.



Poster Presentation : **INOR.P-218**

Inorganic Chemistry

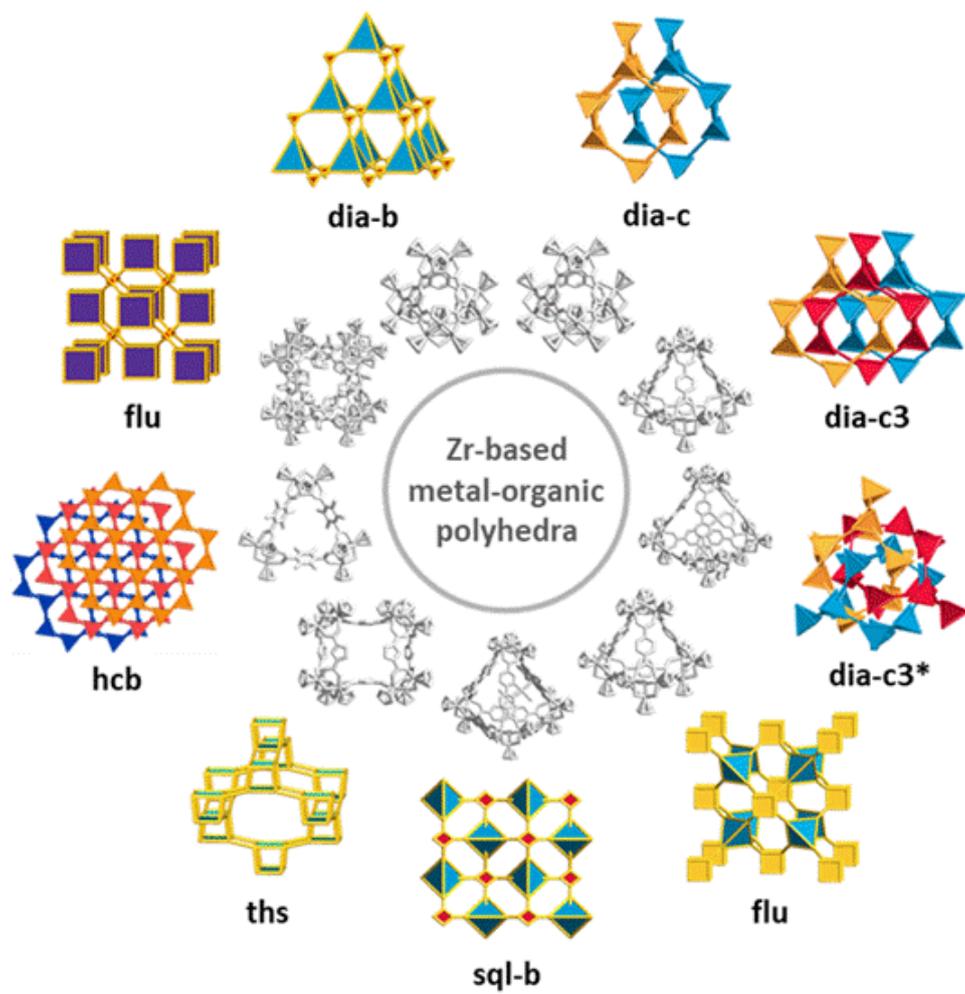
Zoom 5 FRI 16:00~17:00

Topological Packing of Metal-Organic Polyhedra: Bridging Discrete Cages and Extended Frameworks

Jiyeon Kim, Wonyoung Choe*

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

Topological considerations for linking of building blocks, namely reticular chemistry, have accelerated the discovery of new structures by providing a guide and toolbox for anticipated and targeted structures of crystalline materials. Currently, reticular chemistry is focused on strong bonds such as coordination or covalent bonds to connect building blocks. However, we envisioned that the types of interactions could be extended to weaker bonds found in Zr-based metal-organic polyhedra (MOPs), porous molecular solids built from discrete cages and anionic clusters. In this presentation, we introduce topological insight for decoding the solid-state packing of Zr-MOPs (Figure) and highlight the unique dual features of discrete cages and extended frameworks in Zr-MOPs connecting the two fields of porous materials.



Poster Presentation : **INOR.P-219**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Stable Organic Radicals for Cross-Coupling Reactions

Guyoon Jeong, Eunsung Lee*

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

Organic radicals have been of great interest due to their unique reactivity and potential applicability; however, lack of stability continues to limit their application, especially in physiological conditions. For example, well-known aminoxyl radicals have half-life of a few minutes in physiological conditions due to biological redox active reagents, while shielding using polymeric or supramolecular protecting groups increases their half-life up to several hours. Recently, we designed and synthesized a new small molecular organic radical based on 1,2-dicarbonyl scaffold with exceptional stability. The presented radicals showed superior stability over present organic radicals towards physiological conditions (half-life of more than 3000 hours) and even resistant towards harsh conditions such as chemically reducing, oxidizing, acidic, basic conditions, and high temperature, without additional protection. To expand the scope of the 1,2-dicarbonyl, which is stabilized by N-heterocyclic carbenes (NHCs), we introduced the aryl bromide in the radicals and showed palladium-catalyzed cross-coupling reactions with boronic acids. The details will be presented.

Poster Presentation : **INOR.P-220**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Influence of Electronic Environment on the Radiative Efficiency of 9-Phenyl-9*H*-carbazole-Based *ortho*-Carboranyl Luminophores

Seok Ho Lee, Kang Mun Lee*

Department of Chemistry, Kangwon National University, Korea

The photophysical properties of *closo-ortho*-carboranyl-based donor–acceptor dyads are known to be affected by the electronic environment of the carborane cage but the influence of the electronic environment of the donor moiety remains uncertain. Herein, four 9-phenyl-9*H*-carbazole-based *closo-ortho*-carboranyl compounds (**1F**, **2P**, **3M**, and **4T**), in which an *o*-carborane cage was attached to the C3-position of a 9-phenyl-9*H*-carbazole moiety containing various functional groups, were synthesized and fully characterized using multinuclear nuclear magnetic resonance spectroscopy and elemental analysis. Moreover, the solid-state molecular structures of **1F** and **4T** were determined by X-ray diffraction crystallography. Although the *o*-carboranyl compounds were weakly emissive in solution at 298 K, an intense yellowish emission corresponding to an ICT transition involving the *o*-carborane unit were observed in rigid states (in solution at 77 K and in the film state). Theoretical calculations on the first excited states (S_1) of the compounds suggested that the strong emission bands can be assigned to the ICT transition involving the *o*-carborane. Intriguingly, a gradual increase in the Φ_{em} and k_r values for the ICT-based emission of the *o*-carboranyl compounds in the film state was observed as the electron-donating ability of the substituent on the 9-phenyl group increased (–F for **1F** < –H for **2P** < –CH₃ for **3M** < –C(CH₃)₃ for **4T**). These properties strongly indicate that the ICT-based radiative decay process in the *o*-carboranyl compounds was induced by the electron-rich nature of the appended aromatic group. Consequently, the results of this study suggest that the electronic environment of an aryl group linked to an *o*-carborane unit can control the efficiency of radiative decay processes based on ICT transitions.

Poster Presentation : **INOR.P-221**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Activation of Dinitrogen by a Titanium Complex with an Amino Triphenolate Ligand Lead by Geometry Shift

Dae Young Bae, Gunhee Lee, Eunsung Lee*

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

Fixation and functionalization of molecular nitrogen have been of great interest in chemistry for several decades because N₂ has a high potential to convert into an N₁ source. Since the development of Schrock's catalyst, various transition metal complexes have been reported for activating or functionalizing N₂ catalytically. Despite extensive studies of transition metal dinitrogen complexes, transition metal complexes with multi oxygen-based ligands have been less studied for N₂ activation. Herein, we present a titanium dinitrogen complex [$\{(t\text{BuTPA})\text{TiIV}\}_2(\mu\text{-}\eta^1\text{:}\eta^1\text{-N}_2\text{K}_2)(\text{OEt})\text{K}$] (H₂(^tBuTPA) = tris(4,6-di-tert-butyl-2-hydroxybenzyl)amine) supported by a triphenolamine (TPA) ligand for the first time. The complex was characterized by resonance Raman, IR, UV-VIS, and NMR spectroscopy, and single-crystal X-ray diffraction analysis. Most interestingly, the titanium N₂ complex shows asymmetric geometries of titanium ions (TBP-Oh) with bridging nitrogen possibly to minimize a steric demand at metal centers. Finally, N₂ ligand was converted into ammonia in the presence of the titanium N₂ complex with an excess amount of PCy₃HI and KC₈ with 154% yield (per Ti ion).

Poster Presentation : INOR.P-222

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

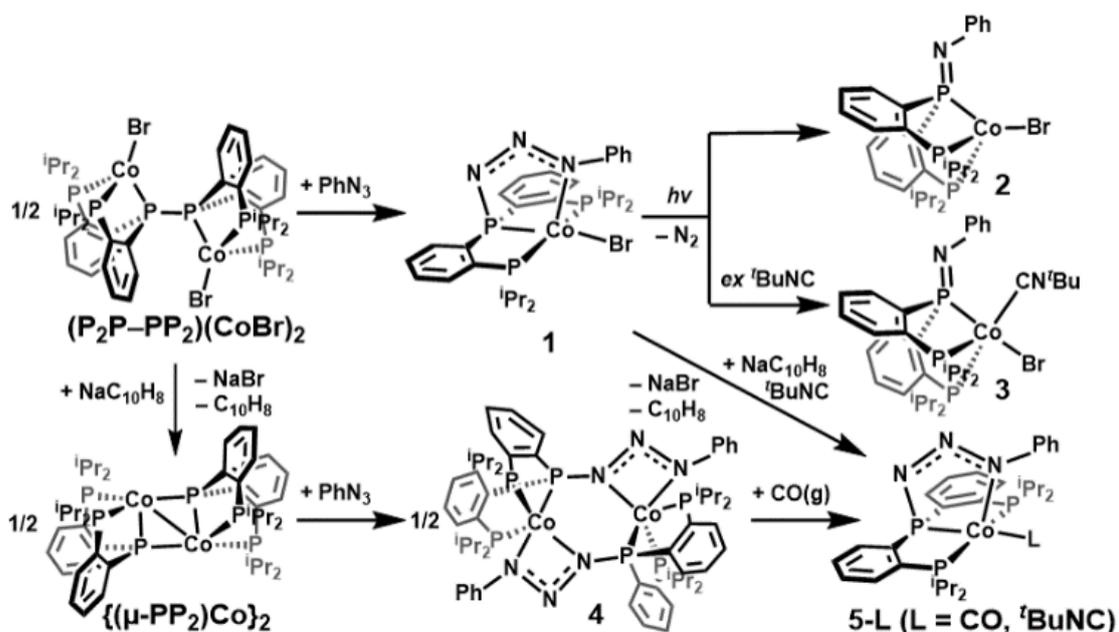
Metal-ligand cooperative azide activation and nitrene group transfer of phosphazido pincer cobalt complex at a Co-P moiety

Yunho Lee*, Kunwoo Lee¹

Department of Chemistry, Seoul National University, Korea

¹Chemistry, Seoul National University, Korea

A Co-P moiety reveals metal-ligand cooperative azide activation and nitrene group transfer after the reaction with alkyl azide. The cobalt-phosphide moiety cooperatively activates azide and the central phosphorus atom operated as an anchoring site for accepting a terminal nitrogen atom of the phenyl azide. To utilize the phosphazido cobalt complex as a nitrene group transfer reagent, CO(g) and its analogue, CNtBu was introduced as a nitrene group acceptor.



Poster Presentation : **INOR.P-223**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

Reductive carbonylation of nitroarenes into carbamates using a heterogeneous Pd catalyst

Sudakar Padmanaban, Yunho Lee^{1,*}, Sungho Yoon^{2,*}

Department of chemistry, Seoul National University, Korea

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

²*Department of Chemistry, Chung-Ang University, Korea*

The reductive carbonylation of nitroarenes in presence of alcohol 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. In this study, a phenanthroline-based heterogeneous Pd-complex, Pd@phen-POP, was synthesized by the solvent knitting of phenanthroline scaffold via the Lewis-acid-catalyzed Friedel-Crafts reaction using dichloromethane as a cross-linker with high porosity and surface area. Pd@phen-POP was demonstrated to be an efficient heterogeneous catalyst for the reductive carbonylation of nitroarenes using nitrobenzene as a model compound. The Pd@phen-POP catalyst showed a high turnover number (TON = 530) and a high turnover frequency (TOF = 45 h⁻¹), with high selectivity (92%) for the carbamate formation during the reductive carbonylation of nitroarenes. The heterogeneous catalyst Pd@phen-POP is recyclable and retains 92% of the original reactivity in the recycling studies.

Poster Presentation : **INOR.P-224**

Inorganic Chemistry

Zoom 5 FRI 16:00~17:00

The selective calcium removal in the cementitious matters

Kyungwon Suh

Korea Atomic Energy Research Institute, Korea

Cementation is an ordinary method to immobilize radionuclides in nuclear wastes. Main element of cementitious matters is calcium. Among several stable calcium isotopes, Ca-40 and Ca-44 is converted to Ca-41 and Ca-45 by the neutron activation reaction. Although it is needed to quantify the amount of Ca-41 because of its long half-life and relatively high mobility in the environment, it interferes to measure Fe-55 and/or Ni-63 by a radiometric method. Therefore, it is required to selectively remove calcium prior to Fe-55 and/or Ni-63 measurement in the cementitious matters. It was confirmed that the precipitation technique with phosphoric acid gave better group separation than the precipitation with oxalic acid. Co-precipitate containing calcium and iron was individually separated by the solvent extraction, which gave that calcium was quantitatively removed from co-precipitate of iron and calcium.

Poster Presentation : **PHYS.P-225**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Isotope effects in the collision of α -chlorotoluene with H₂ and D₂

Sang kwon Lee, Jongbaik Ree^{1,*}

Department of Chemistry Education, Chonnam National University, Korea

¹*Department of Chemical Education, Chonnam National University, Korea*

We have studied the vibrational relaxation of excited α -chlorotoluene and dissociations of C-H_{ring} and C-Cl bonds in the α -CT + H₂/D₂ collision reactions at 300 K using classical trajectory procedure. The vibrational energy loss of excited α -CT by the collision of the ground-state H₂/D₂ is small, but it increases with increasing the total vibrational excitation, E_T. The amount of energy loss is significantly larger in α -CT + D₂, especially over 30,000 cm⁻¹ of E_T. On the contrary, the vibrational relaxation of α -CT is mainly due to the C-Cl vibrational decay. Furthermore, the heavier D₂ induces stronger perturbation on α -CT, thus enhancing the vibrational relaxation process of α -CT. In both α -CT + H₂ and α -CT + D₂ collisions, the contribution of the V-T process is dominant to the vibrational decay of α -CT, whereas the V-V and V-R processes are inefficient in both collisions. Dissociation probabilities in both collisions are low but rise very rapidly with increasing the total vibrational excitation. The probability of the C-Cl bond dissociation is lower than the C-H_{ring} bond dissociation nearly below 70,000 cm⁻¹ of E_T, because the probability of that the C-Cl bond gains the sufficient energy to dissociate is low compared to the C-H_{ring} bond. The dissociation probabilities of C-H_{ring} and C-Cl bonds in the α -CT + D₂ collision are found to be higher than the α -CT + H₂ collision due to more efficient perturbation. The present values are significantly lower than those of toluene + N₂/O₂, while they are comparable with those for toluene + H₂/D₂ collisions.

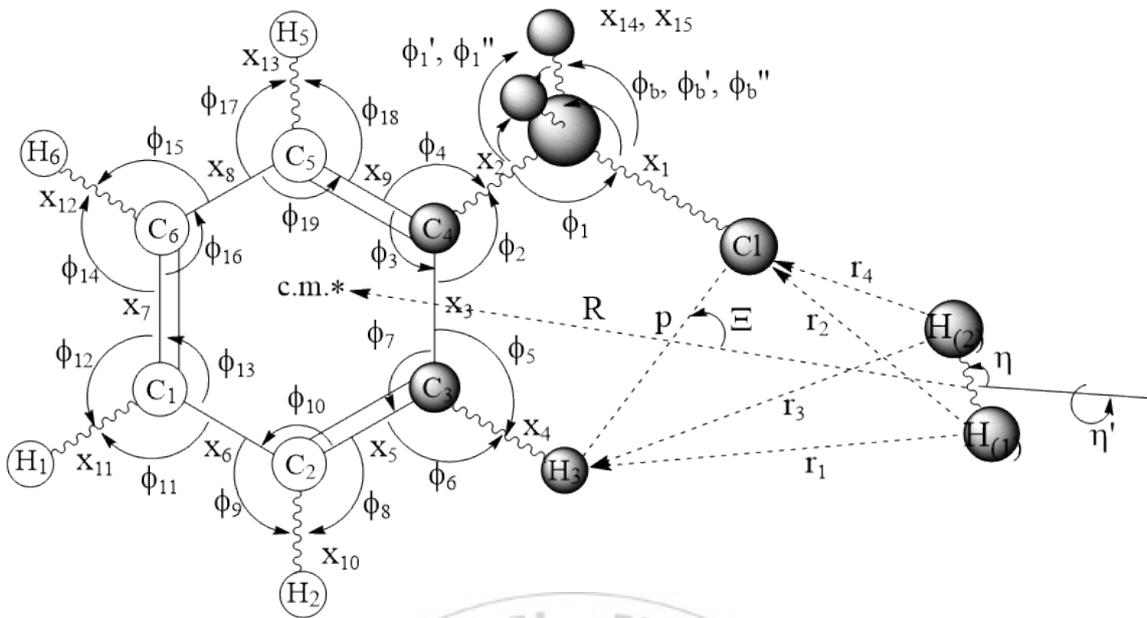


FIG. 1

Poster Presentation : **PHYS.P-226**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

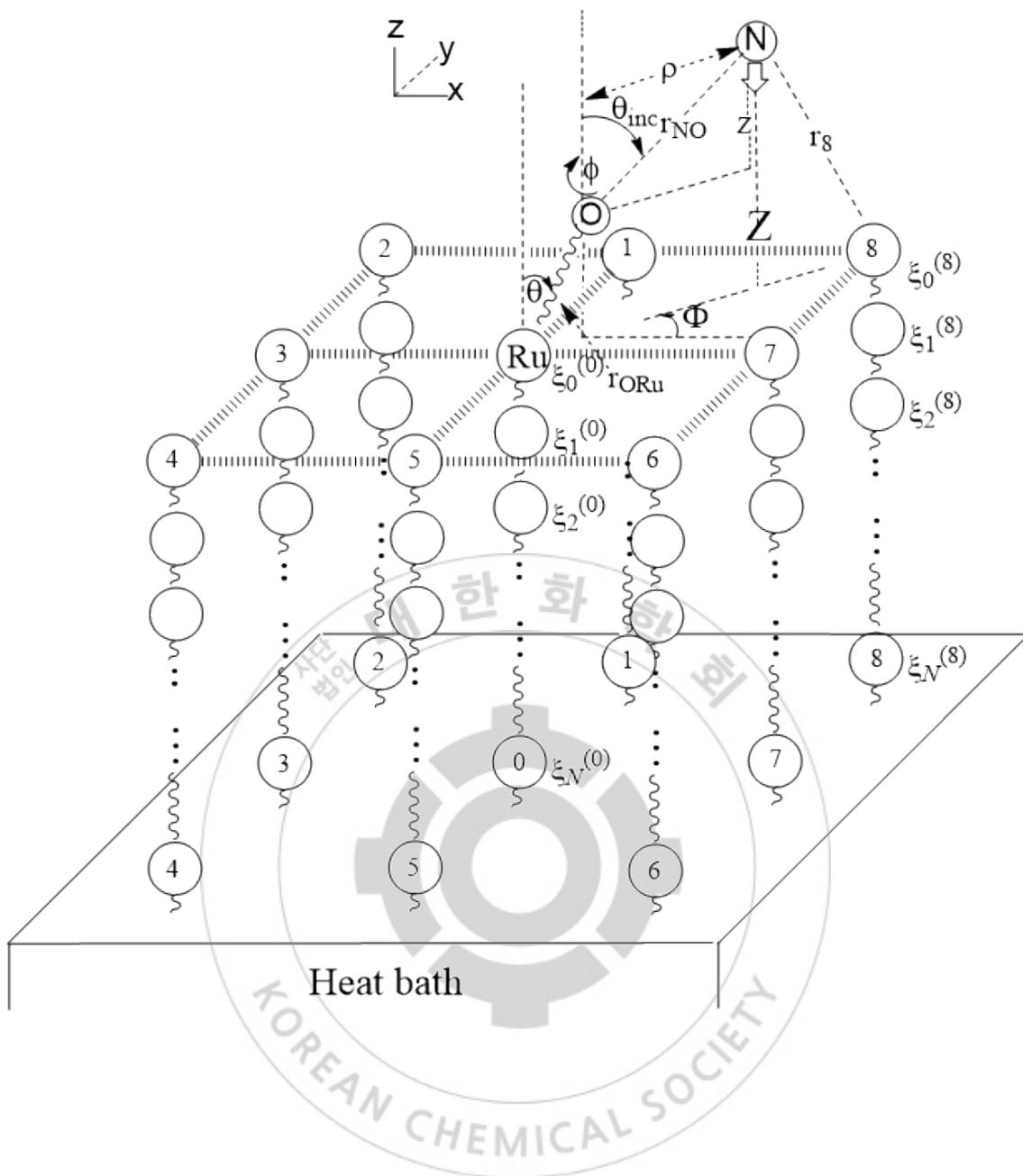
Reaction of Atomic Nitrogen with Chemisorbed Oxygen Atoms on a Ru(0001) Surface

Kyoung Chul Ko, Jongbaik Ree^{1,*}

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¹*Department of Chemical Education, Chonnam National University, Korea*

We have calculated the probability of NO formation and energy deposit of the exothermic reaction energy of the newly formed NO, particularly in its vibrational motions, in the gas-surface reaction $\text{N(g)} + \text{O(ad)/Ru(0001)} \rightarrow \text{NO(g)} + \text{Ru(0001)}$. The reaction probability at on-top site of Ru(0001) surface is about 0.01 at gas temperature 1800 K and surface temperature 300 K. On the contrary, the reaction probability at hollow site is slightly greater than on-top site. For both cases, the vibrational and translational motions of product NO share the most of the reaction energy. Increasing the initial vibrational state of the adsorbed O atom from the ground state to $v = 1, 2$ and 3 causes only slight variation of the partitioned energies shared by NO product. However, strong vibrational excitation in NO leads to a vibrational population inversion. The amount of energy propagated into the bulk solid phase is calculated as a negative value, which means the energy transfer from the surface to the desorbed product. The dependence of reaction probabilities and energy distributions on surface temperature is found to be weak in the range of $0 - 1500$ K for surface temperature.



Poster Presentation : **PHYS.P-227**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Vibrational Energy Transfer to the Hydrogen Bond in the Uracil-Water Complexes

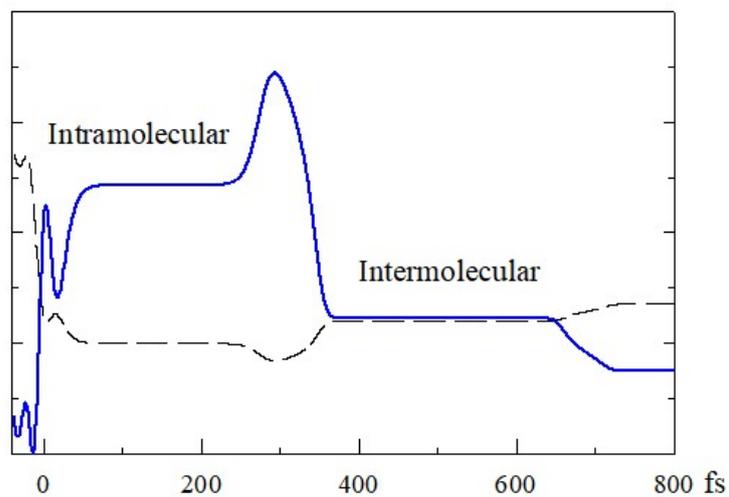
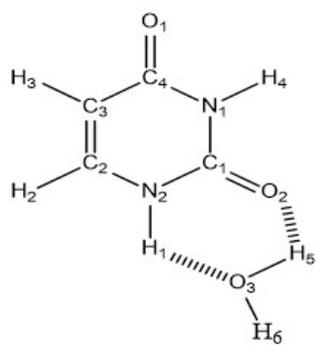
Kyoung Chul Ko, Jongbaik Ree^{1,*}, Hyung Kyu Shin²

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In the uracil-water complex, the vibrational energy initially stored in the OH($\nu=1$) stretch efficiently transfers to the first overtone-bending mode under a near-resonant condition. The relaxation of the overtone vibration redistributes its energy to uracil and the two hydrogen bonds in the intermolecular zone, which consists of the OH bond and the bonds between nearby C, N, O and H atoms of uracil. The uracil NH bond and the hydrogen bond it formed with the water molecule, N-H...O, store the major portion of the energy released by the relaxing bending mode, thus forming a localized hot band in the intermolecular zone. Energy transfer to the bonds beyond the zone is found to be not significant. Impressed by efficient near-resonant energy transfer pathways, the time evolution of the centers of mass distance shows the phenomenon of beats. One global and two different local minima energy structures are considered. The results of energy transfer do not significantly differ, suggesting the two hydrogen bonds in all three structures have similar contributions to the energy transfer.



Poster Presentation : **PHYS.P-228**

Physical Chemistry

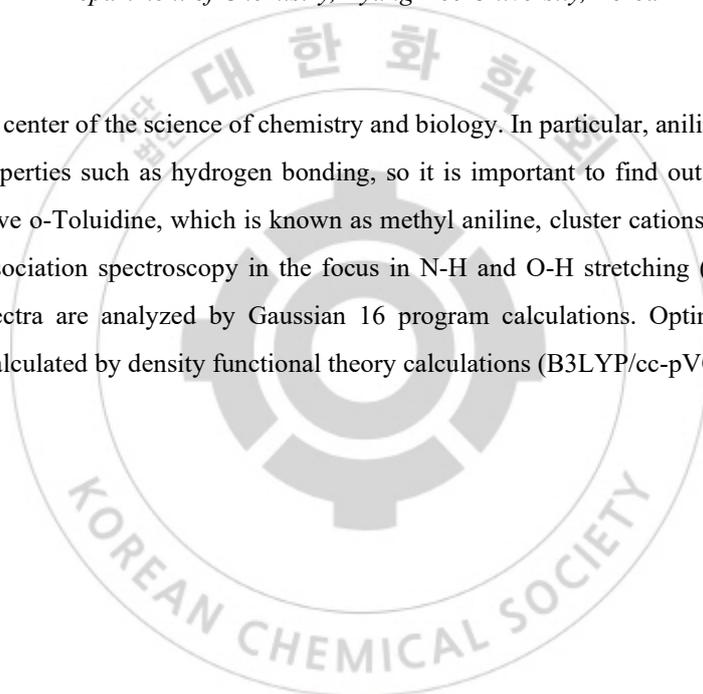
Zoom 6 FRI 15:00~16:00

Structures of o-Toluidine-Water (oTWn) Cluster Cation ($n \leq 6$)

BongGyu Jeong, Dong Hun Hwang, Jae Kyu Song, Seung Min Park*

Department of Chemistry, Kyung Hee University, Korea

Cluster ions are the center of the science of chemistry and biology. In particular, aniline derivative clusters have important properties such as hydrogen bonding, so it is important to find out their characteristics. Herein, size-selective o-Toluidine, which is known as methyl aniline, cluster cations are characterized by infrared action dissociation spectroscopy in the focus in N-H and O-H stretching (2800 ~ 3800 cm^{-1}). Infrared action spectra are analyzed by Gaussian 16 program calculations. Optimized structures and frequencies were calculated by density functional theory calculations (B3LYP/cc-pVQZ).



Poster Presentation : **PHYS.P-229**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Observation of vibronic emission spectrum of jet-cooled 4-chloro-m-xylyl radical

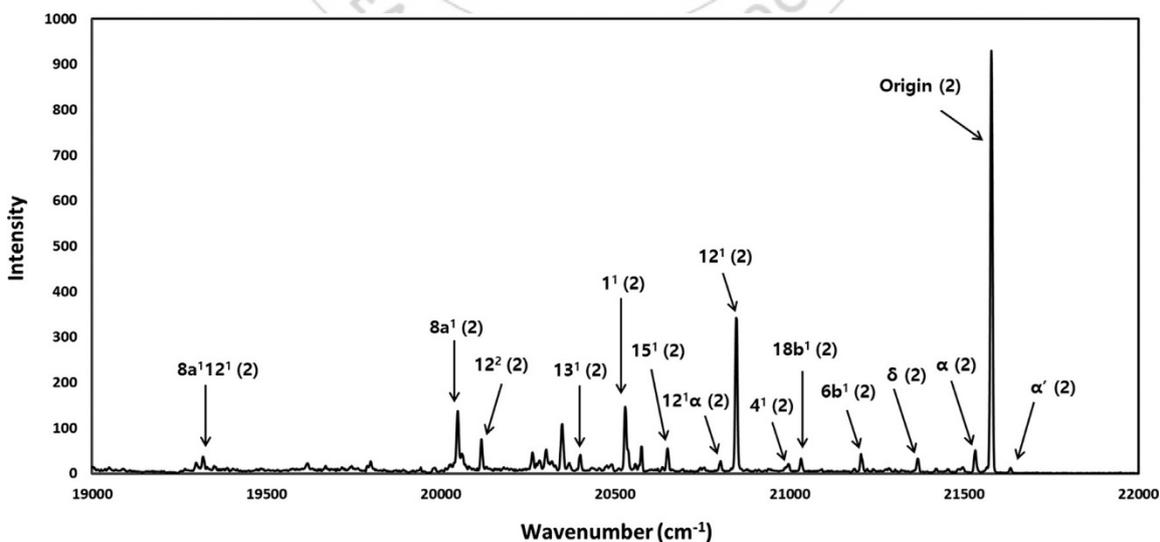
Changsoon Huh*, Kim Subin¹, Jungwon Han², Jaehyuck Kim²

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¹*Apply Chamistry, Dong-Eui University, Korea*

²*Dong-Eui University, Korea*

We report the vibronic emission spectrum of 4-chloro-m-xylyl radical using a long-path monochromator in acorona-excited supersonic expansion (CESE). By the precursor 4-chloro-m-xylene, we identified 4-chloro-m-xylyl from the two isomeric benzyl-type radicals analyzing a Franck-Condon simulation and ab initio calculations. From an analysis of the vibronic emission spectrum of the 4-chloro-m-xylyl radical, the D1→D0 electronic transition energy was confirmed and the assignments of vibrational frequencies were accomplished in the ground state.



Poster Presentation : **PHYS.P-230**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Use of Fe-oxide/Al₂O₃ as an oxidation catalyst to treat NH₃ and H₂S

Jiyeon Choi, Soong Yeon Kim, Young Dok Kim*

Department of Chemistry, Sungkyunkwan University, Korea

In our previous studies, Fe-oxide/Al₂O₃ structure, prepared by temperature regulated chemical vapor deposition(TR-CVD) had shown high performances on removal of various harmful gases such as CO, VOCs and NO in our previous studies. In the present work, Fe-oxide/Al₂O₃ was used for the removal of NH₃ and H₂S gases which are particularly odorous among other types of harmful gases that were not previously studied with, and we show that Fe-oxide/Al₂O₃ can also efficiently eliminate NH₃ and H₂S. In case of NH₃, 2% of NH₃ could be all removed above the reaction temperature of 450 oC, and during the removal reactions, only N₂ gas was generated as reaction product without formation of nitrogen oxides. Then, adsorption of NH₃ on Fe-oxide/Al₂O₃ and their thermal desorption process was repeatedly performed which resembles the practical operating conditions. The adsorption capacity of Fe-oxide/Al₂O₃ could be fully recovered by 500 oC of thermal treatment, and during this thermal treatment, adsorbed NH₃ was either desorbed as NH₃ or N₂ gas. A differential temperature controlled catalysis system was proposed which could effectively reduce emission of NH₃ during the thermal desorption process of NH₃. Removal mechanism of NH₃ on Fe-oxide/Al₂O₃ and the role of Fe-oxide on catalytic reactions were tracked by operando FT-IR analyses. The similar adsorption and thermal desorption method as in NH₃ was applied to H₂S gas (2000 ppm). Majority of adsorbed H₂S either desorbed as elemental sulfur or remained on the surface as in oxide forms during the thermal desorption process and small portion of the adsorbed H₂S was desorbed as SO₂. Removal mechanism of H₂S on Fe-oxide/Al₂O₃ and the role of Fe-oxide on catalytic reactions were elucidated via XPS analyses.

Poster Presentation : **PHYS.P-231**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Photocatalytic abatement of NO_x by Fe loaded TiO₂ particles mixed with surface hardening agent under visible light irradiation

Shufang Zhao, Soong Yeon Kim, Saqlain Shahid, Young Dok Kim *

Department of Chemistry, Sungkyunkwan University, Korea

Cost effective visible light driven Fe-TiO₂ photocatalyst was prepared by loading Fe into commercially available rutile TiO₂ using temperature regulated chemical vapor deposition (tr-CVD) method and then subsequent annealing at 375 °C. This Fe-TiO₂ photocatalyst was measured for photocatalytic degradation of NO_x under visible light irradiation at relative humidity of 50%. The experimental results showed that, this Fe doped TiO₂ was highly efficient for the removal of NO compared to pristine TiO₂. When the Fe-TiO₂ photocatalyst was combined with surface hardening agent to immobilize its particles on cement block substrate, although the composite of Fe-TiO₂ with hardening agent on the cement block showed lower NO removal, yet the NO₃⁻ selectivity during oxidation of NO was increased compared to Fe-TiO₂ used alone. Moreover, when different contents of Fe-TiO₂ particles (0, 5, 9, 11, and 23%) mixed with hardener were coated on cement block by using watering method, the photocatalytic removal of NO was increased as the Fe-TiO₂ content was increased from 0 to 11%, whereas the NO removal was slightly decreased as content of Fe-TiO₂ (23%) was increased further. The study suggests that optimum content of Fe-TiO₂ particles with hardening agent on cement block is one of the quite important factors for the enhanced photocatalytic oxidation of NO in real applications.

Poster Presentation : **PHYS.P-232**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Operando Raman and UV-Vis spectroscopic studies of the coloring and bleaching mechanism of self-powered photochromic devices

So Yeon Chun, Minhaeng Cho, Kyungwon Kwak*, Han-Kyu Choi^{1,*}

Department of Chemistry, Korea University, Korea

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

Smart windows, which are drawing attention as an important part of energy-efficient building design, must be able to change colors homogeneously on a large-scale while controlling the intensity of daylight. However, the electrochromic devices (ECDs) studied mainly have limitations due to technical requirements. Among candidates suitable for smart windows, photochromic devices (PCDs) have great potential to utilize as color-switchable windows. In a PCD, the intercalation/deintercalation of Li-ions during the coloring/bleaching process plays an important role in the color-switching performance of the device. In this study, we propose a predictive mechanism for PCD using operando Raman and UV-Vis spectroscopy. The spectral shift of the characteristic peaks of tungsten oxide (WO_3) observed in the time-resolved Raman spectra indicates the intercalation/deintercalation of Li-ions associated with specific sites within the tunnel present in hexagonal WO_3 lattice. This study improves the understanding of the kinetics and efficiencies of the coloring/bleaching process that determines the photochromic performance and opens up the field of research for the development of smart windows applications.

Poster Presentation : **PHYS.P-233**

Physical Chemistry

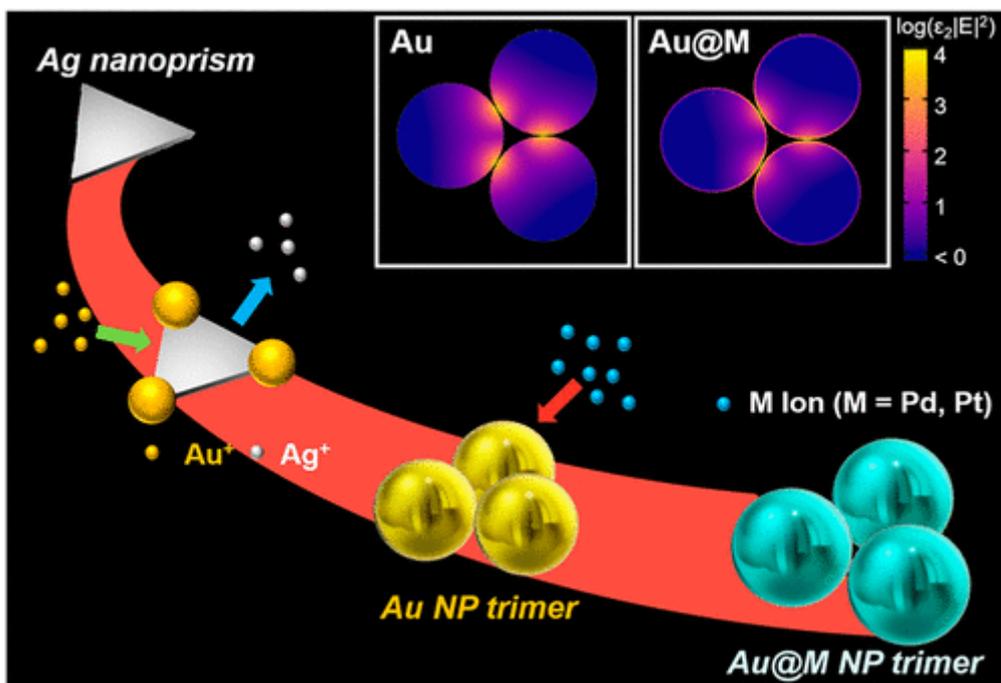
Zoom 6 FRI 15:00~16:00

Light-to-Chemical Energy Conversion in Core-Shell Bimetallic Nanoparticle Trimers

Younghyun Wy, Sang Woo Han*

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

Incorporation of catalytically active materials into plasmonic metal nanostructures can efficiently merge the reactivity and energy-harvesting abilities of both types of materials for visible light photocatalysis. Herein, we explore the influence of electromagnetic hotspots in the ability of plasmonic core-shell colloidal structures to induce chemical transformations. For this study, we developed a synthetic strategy for the fabrication of Au nanoparticle (NP) trimers in aqueous solution through fine controlled galvanic replacement between Ag nanoprisms and Au precursors. Core-shell Au@M NP trimers with catalytically active metals (M = Pd, Pt) were subsequently synthesized using Au NP trimers as templates. Our experimental and computational results highlight the synergy of geometry and composition in plasmonic catalysts for plasmon-driven chemical reactions.



Poster Presentation : **PHYS.P-234**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Effects of the anion structure on the diffusion mechanism of the lithium ion (Li^+) in ionic liquids

Chung Bin Park, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Mixture of alkali metal ion salts and ionic liquids has been attracted as a safe electrolyte for Li^+ battery. As the concentration of alkali ion increases, however, the electrolyte shows poor conductivity due to aggregations between anions and Li^+ . Furthermore, to be a better electrolyte for Li^+ battery, Li^+ should diffuse solely instead of collective and associated diffusion with anions. In this work, we investigate how the structure of anions affects the associated diffusion of Li^+ in the salt mixtures by molecular dynamics simulation. We employ five kinds of salt mixture with five different anions, $\text{Li}_x\text{MMIM}_{1-x}\text{A}$ ($\text{A}^- = \text{Cl}^-, \text{BF}_4^-, \text{PF}_6^-, \text{FSI}, \text{TFSI}$, MMIM = 1,3-dimethyl imidazolium). To investigate the relations between anion structures and diffusion mechanisms of Li^+ , we calculate distinct (correlated) part of displacement and transference number of Li^+ . From our results, diffusions of Li^+ show low correlation with that of sulfonyl imide anions (TFSI, FSI), while they show higher correlations with diffusion of spherical shape anions ($\text{Cl}^-, \text{BF}_4^-, \text{PF}_6^-$). This indicates the decoupling between diffusion of Li^+ and that of sulfonyl imide anions. Li^+ can escape from the solvation shell by the rotations of S=O bond as Li^+ is solvated with oxygen atom of S=O. Especially, fast rotational motion of S=O of FSI enable Li^+ to move to neighbor anion easily. As a results, Li^+ shows highest transference number despite of high viscosity of the $\text{Li}_{0.5}\text{MMIM}_{0.5}\text{FSI}$.

Poster Presentation : **PHYS.P-235**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Two-dimensional Infrared Spectroscopy reveals the Structural and Dynamics Information of poly(ethylene carbonate) based solid polymer electrolytes

Seoeun Shin, Chaiho Lim, Kyungwon Kwak*, Minhaeng Cho*

Department of Chemistry, Korea University, Korea

Solid polymer electrolytes (SPEs) are one of prospective solid electrolytes for the all-solid-state batteries because SPEs have advantages towards to conventional liquid-type electrolytes in terms of safety issues and flexibility of material. However, SPEs are suffering from their low ionic conductivity. Many researchers have investigated various systems such as polymer blend, block copolymer, and polymer-in-salt system to improve the performance, however SPEs still have many limitations. In order to understand the fundamental causes of these problems, research at a microscopic level is necessary. Infrared spectroscopies are one of the tools for a microscopic level study of SPE systems. Furthermore, ultrafast time-resolved infrared spectroscopy can provide not only more detailed structural information, but also picosecond dynamics of SPE systems. Among many polymer hosts for SPEs, polyalkylene carbonates are proper polymer hosts for IR study because they have carbonyl stretch modes which are sensitive infrared probes for detecting changes of surroundings. In this study, structures and dynamics of SPEs composed of polyethylene carbonate (PEC) and lithium perchlorate were investigated using Fourier-transform infrared (FTIR) spectroscopy and two-dimensional infrared (2DIR) spectroscopy. We acquired structural information such as Li⁺ ion coordination number and dimer structure of polymer chains with these IR spectroscopies.

Poster Presentation : **PHYS.P-236**

Physical Chemistry

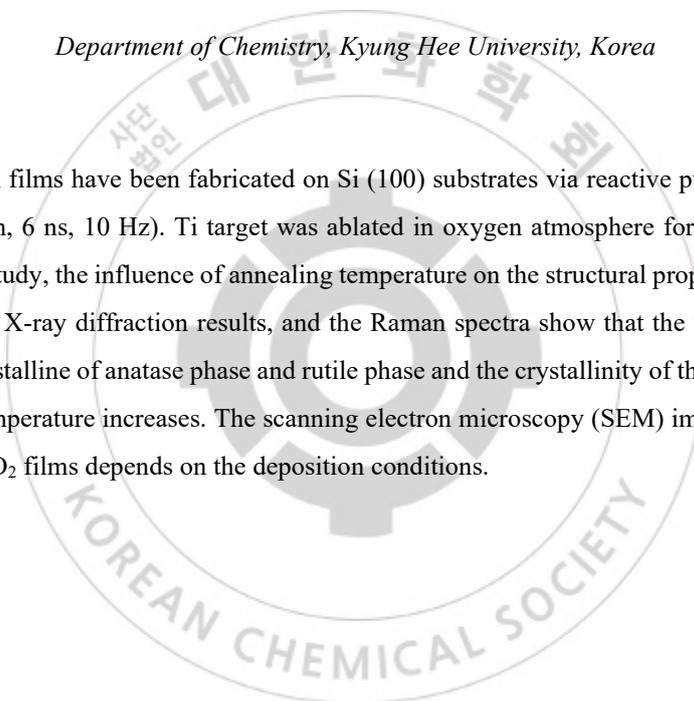
Zoom 6 FRI 15:00~16:00

Effect of annealing temperature on the structural characteristics of TiO₂ films fabricated by reactive pulsed laser deposition

Dong Hun Hwang, Bong Gyu Jeong, Jae Kyu Song, Seung Min Park*

Department of Chemistry, Kyung Hee University, Korea

Titanium oxide thin films have been fabricated on Si (100) substrates via reactive pulsed laser deposition (Nd:YAG: 1064 nm, 6 ns, 10 Hz). Ti target was ablated in oxygen atmosphere for reactive pulsed laser deposition. In this study, the influence of annealing temperature on the structural properties of the thin film was discussed. The X-ray diffraction results, and the Raman spectra show that the film deposited on the substrate is polycrystalline of anatase phase and rutile phase and the crystallinity of thin film was improved as the annealing temperature increases. The scanning electron microscopy (SEM) images indicate that the grain size of the TiO₂ films depends on the deposition conditions.



Poster Presentation : **PHYS.P-237**

Physical Chemistry

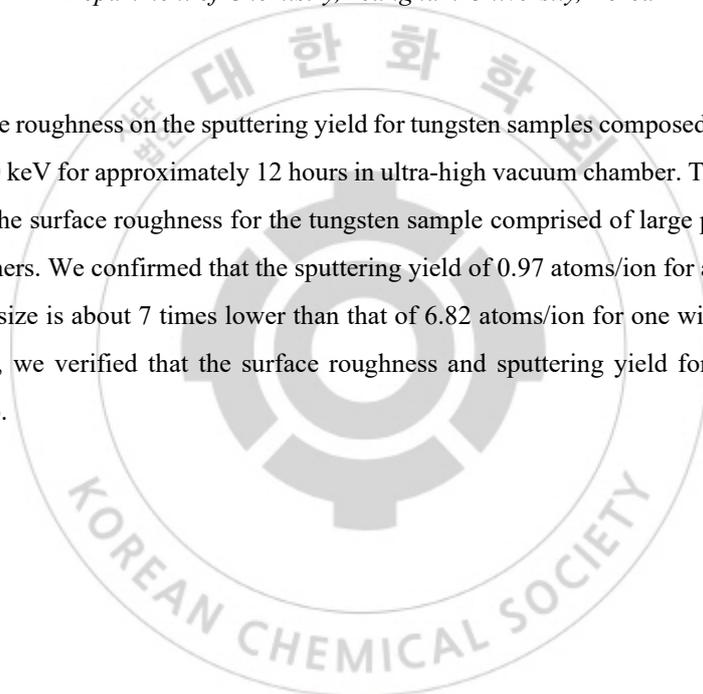
Zoom 6 FRI 15:00~16:00

Effect of surface roughness on sputtering yield for tungsten

Tae Hyun Kwon, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

The effect of surface roughness on the sputtering yield for tungsten samples composed of different particles sizes of $+$ ions at 2.0 keV for approximately 12 hours in ultra-high vacuum chamber. The data of the surface profiler show that the surface roughness for the tungsten sample comprised of large particle size is higher compared to the others. We confirmed that the sputtering yield of 0.97 atoms/ion for a tungsten pellet with the largest particle size is about 7 times lower than that of 6.82 atoms/ion for one with the lowest particle size. Consequently, we verified that the surface roughness and sputtering yield for tungsten exhibit an inverse relationship.



Poster Presentation : **PHYS.P-238**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Lasing of heterostructure AlGa_N/Ga_N/InGa_N nanorods

Sungjae Won, Jae Kyu Song*

Department of Chemistry, Kyung Hee University, Korea

One-dimensional semiconductor nanomaterials, such as nanowires and nanorods, can serve as both optical cavity and gain medium, which are suited for nanoscale lasers. The nanorod lasers have been reported for several homogeneous binary semiconductors, including GaN, ZnO, and CdS. In addition, ternary semiconductor nanorods can change the composition ratio to control the properties such as the band gap energy. We investigate the optical properties of AlGa_N/Ga_N/InGa_N heterostructure nanorods and observe the lasing of GaN and InGa_N. Adding AlGa_N and InGa_N layers causes the difference in the mode spacing of GaN lasing, which is explained by light-matter interactions. The amplified spontaneous emission of InGa_N is explained by Fabry-Pérot optical cavity model.

Poster Presentation : **PHYS.P-239**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Simple Synthesis of Side-by-Side Ag-AuNPs/Y₂SiO₅: Pr³⁺ Up-conversion Nanophosphors 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, Y₂SiO₅:Pr³⁺, converts visible light into UV light (280 – 340 nm). However, this material has low conversion efficiency, limiting its application. In this report, a side-by-side structure including up-converting phosphors combined with Ag NPs were developed, allowing the enhancement of the up-converting efficiency by using Ag NPs as light intensity amplification. Visible light intensity was enhanced by Ag NPs nearby, absorbed to the up-conversion material with higher efficiency. The materials were characterized primarily by TGA, XPS, TEM, EDS showing the clear side-by-side structure and underlying formation mechanism.

Poster Presentation : **PHYS.P-240**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Copper Tin Bimetallic Alloy Combining with Reduced Graphene Oxide, Poly(4-vinylpyridine), and Nafion as Cathode for Efficient Photoelectrochemical CO₂ Reduction Reaction

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Chemistry, Sogang University, Korea

¹*Department of Chemistry, Sogang University, Korea*

CO₂ level is increasing in the atmosphere nowadays and it has caused climatic problem such as global warming. Conversion of CO₂ into renewable energy sources is not only decreases the CO₂ concentration in the atmosphere but also stores renewable energy. The electrochemical CO₂ reduction reaction (CO₂RR) have been studied by combining metal such as Sn with Cu to improve the activity and selectivity of CO₂RR. Copper tin nanoparticles were developed by phase and structure engineering to get core-shell structure as cathode and BiVO₄ as photoanode for photoelectrochemical (PEC) CO₂RR. Moreover, reduced graphene oxide (rGO) was coated on the surface of Cu_x-Sn_y to have sequential multi-electron shuttling process. Then, poly(4-vinylpyridine) or PVP was coated on the surface of rGO/Cu_x-Sn_y to do CO₂ adsorption and activation to decrease activation energy of rate determining first electron transfer and reduction reaction energy for CO₂RR. Pyridine molecules have been used as a catalyst to reduce the activation energy of the CO₂RR. Nafion (Naf) as proton-conductive polymer was coated on the surface of PVP/rGO/Cu_x-Sn_y to make one pot reaction of proton-coupled sequential multi-electron transfer from rGO to CO₂ reduction site due to its extremely high proton conductivity and negligible electron conductivity. This work suggests new creative strategy to fabricate multi-functional hybrid composite layer electrode with high faradaic efficiency and high selectivity of CO₂RR to produce liquid product.

Poster Presentation : **PHYS.P-241**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Reaction Control Effect by the Halide Exchange of Cesium Lead Halide Perovskite Nanocrystals through the introduction of PbSO₄-Oleate Capping

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Department of Chemistry, Yeungnam University, Korea

¹*Department of Chemistry, Duksung Women's University, Korea*

The selective control of halide ion exchange has an important role in determining the bandgap and composition of nanocrystals in metal halide nanocrystals (NCs). To selectively control the halide ion exchange, CsPbX₃ (X = Cl-, Br- and I-) NCs were self-assembled with PbSO₄-oleate to form a peapod-like form. Taking advantage of these NCs distinct absorption and bright luminescence properties, in situ UV-Vis. absorption and fluorescence spectroscopy tools can be utilized to monitor the changes in the NCs bandgap and composition over time. It can be seen that unlike the fast anion exchange of non-capped NCs, capped nanocrystals retain their respective fluorescence and absorption properties for a longer period of time. In addition, the halide exchange depends on the reaction time to change the number of peapod layer coverage in NCs. In order to track halide ion exchange, the application range of NCs peapod was changed and measured according to the application range through in-situ UV-Vis. absorption/photoluminescence spectroscopies. Time adjustment of the peapods self-assembly process allows selective control of the bandgap and composition ratio of the nanocrystals by controlling the rate of the halide exchange reaction. These results can be attributed to white-LEDs, photovoltaic cells, and photocatalysts using the divalent composition of the CsPbX₃ NCs for alternative structural designs.

Poster Presentation : **PHYS.P-242**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Defect-selective atomic layer deposition of ZnO for wafer-scale single-domain-like graphene with enhanced electronic transport properties

Sung Ho Yu, Myong Mo Sung, Myong Mo Sung*

Department of Chemistry, Hanyang University, Korea

Large-area graphene films produced by means of chemical vapor deposition (CVD) are polycrystalline and thus contain numerous grain boundaries that can greatly degrade their performance and produce inhomogeneous properties. A better grain boundary engineering in CVD graphene is essential to realize the full potential of graphene in large-scale applications. Here, we report a defect-selective atomic layer deposition (ALD) for stitching grain boundaries of CVD graphene with ZnO so as to increase the connectivity between grains. In the present ALD process, ZnO with a hexagonal wurtzite structure was selectively grown mainly on the defect-rich grain boundaries to produce ZnO-stitched CVD graphene with well-connected grains. For the CVD graphene film after ZnO stitching, the inter-grain mobility is notably improved with only a little change in the free carrier density. We also demonstrate how ZnO-stitched CVD graphene can be successfully integrated into wafer-scale arrays of top-gated field-effect transistors on 4-inch Si and polymer substrates, revealing remarkable device-to-device uniformity.

Poster Presentation : **PHYS.P-243**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Charge accumulation phenomenon at new energy level due to π - π stacking of self-assembled monolayer

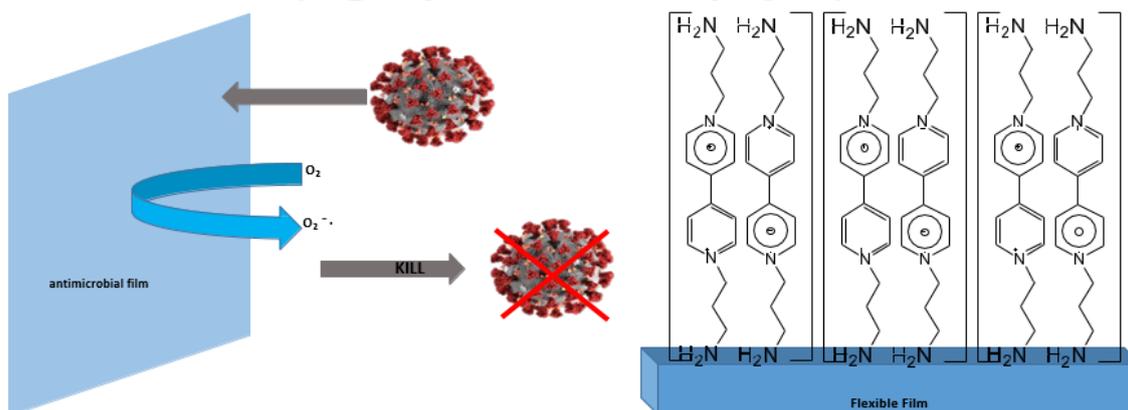
Sumi Seo, Soo Jeong Lee¹, Sung-Hwan Han^{2,*}, Seog Joon Yoon^{*}

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²*Department of Chemistry, Hanyang University, Korea*

As various social problems arise due to COVID-19 pandemic, the development of various products to prevent the spread of pathogens is being activated. We are studying how anti-pathogen works with detailed mechanism, and whether peroxide formation is an important factor in the mechanism about the anti-pathogen. We firstly aimed to study what are the effects of sunlight and/or visible light irradiation, and we will elucidate formation of superoxide through electron transfer from the energy level generated by π - π stacking.



Poster Presentation : **PHYS.P-244**

Physical Chemistry

Zoom 6 FRI 15:00~16:00

Influence of Defects and their Mobility on the Dynamic Heterogeneity in Organic Ionic Plastic Crystals

Hyungshick Park, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Organic ionic plastic crystals (OIPCs) are the ionic crystals, which have a long-range translationally ordered structure. Ions in plastic crystals, however, have extra rotational degree of freedom even in solid phase. Such orientational motions of ions may facilitate the diffusion of dopants like lithium ions. Hence, OIPCs have been widely investigated as good candidates for solid electrolytes. Recent experimental studies showed that the number and volume of defects are strongly correlated to the conductivity of OIPCs. In addition, theoretical studies suggested that the presence of defects facilitates the heterogeneous dynamics in OIPCs: the diffusion of some ions was quite fast while other ions hardly diffuse. Such dynamic heterogeneity would be a key to the ion transport mechanism in solid state electrolyte. In this work, we investigate the translational and rotational dynamic heterogeneity of OIPCs with defects. We conduct atomistic molecular dynamics simulations of 1,3-dimethylimidazolium hexafluorophosphate ([MMIM][PF₆]) with 0.39 mol% defects (one pair of a cation and an anion removed from 4X4X2 supercell). At low temperature, a pair of vacancies show hopping motions toward each other until the formation of a charge-neutral cluster. At high temperature, two vacancies diffuse together and loosely connected to each other by electrostatic interaction. We conclude that the hopping of vacancy is correlated strongly with the translational motion of ions and strengthens the translational dynamic heterogeneity of [MMIM][PF₆]. The rotation of ions is also facilitated when the ions are close to vacancies such that rotational motions become spatially heterogeneous.

Poster Presentation : **PHYS.P-245**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Tracer dynamics reveals the structural order of glass-forming liquids.

Dong jae Chun, Bong June Sung^{1,*}

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¹*Department of Chemistry, Sogang University, Korea*

When glass-forming liquids cool down to glass transition temperature, its dynamics not only drastically slows down but also becomes highly heterogeneous. Even though glasses are ubiquitous in our daily life, it remains an unsolved problem whether the glass transition would be a kinetic trap or a thermodynamic phase transition. Besides, the presence of the structural order that is believed to build the solidity of glasses in recent research results has been a topic of study for decades. It is, however, a non-trivial task to identify and analyze the structural order in glass-forming liquids. Here, we suggest an in-direct way of scrutinizing the local structural order by introducing tracers as stand-ins. We perform molecular dynamics simulations for two-dimensional (2D) polydisperse and binary colloids with tracers. Both two systems are well known to form glasses but have different nature. As being glasses, polydisperse colloids form hexagonal bond orientational order, while binary colloids go against the order. We confirm the translation-rotation decoupling of diamond tracers is more drastic than that of square tracers in polydisperse glasses. Diamond tracers have to overcome a large free energy barrier and break the structural commensurateness in polydisperse media. On the other hand, in binary media, there is no difference in the degree of translation-rotation decoupling between diamond and square tracers. Our results confirm tracer dynamics reflects the hidden structural order of polydisperse glass-forming liquids. It also informs us of the feature of binary glasses that its structural order has nothing to do with hexagonal bond orientational order. We expect our proxy methodology to apply to many other scientific questions.

Poster Presentation : **PHYS.P-246**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

A simulation study on an effect of flexibility of polymer chains on the spatial arrangement and dynamics of a ring polymer in thin linear polymer film

Jong Ho Choi, Bong June Sung*

Department of Chemistry, Sogang University, Korea

A polymer without chain ends, a ring polymer, is subject to small conformation fluctuations and hardly likely to entangle other ring chains; therefore, it can be an easy-to-process polymeric material with low viscosity. When the ring chain is mixed with linear polymer chains, the linear chains penetrate through the ring and hinder the diffusion of it. In addition, a recent study showed that ring chains were not uniformly distributed when polymer films of ring and linear polymer mixtures were prepared (Phys. Rev. Lett. 118, 167801 (2017)). For these reasons, the diffusion of ring polymers in polymer film is much more complicated than in the bulk polymer. In this work, we perform molecular dynamics simulations for the thin polymer films of a single ring polymer chain and linear polymers in order to investigate the ring chain diffusion. Ring and linear polymer chains are made of monomers of identical mass and diameter. In addition, we introduce two different type of polymer chains with different rigidity to investigate whether the rigidity of polymer chain affect its spatial arrangement and diffusion. We find that the flexible ring polymer chain is located in the interfacial region of polymer film where the diffusion of polymer is faster than the bulk polymer while rigid one is in the central region. Therefore, the rigidity of the ring chain affects the diffusion of it although diffusion in bulk polymer melt hardly depends on the rigidity of ring. Although polymer chains with different rigidity have different potential energy, the energy differences of polymer chain in interfacial and central region of the film does not vary with the rigidity of the chain. Thus, it can be assumed that the spatial arrangement of the ring polymer in the film is entropically driven.

Poster Presentation : **PHYS.P-247**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Elucidation of Water-stable CsPbBr₃@SiO_x Perovskite Quantum Dots Formation Mechanism

Soo Jeong Lee, YouJeong Lee, Seog Joon Yoon^{1,*}

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For the next-generation solar cell, the energy payback is also important factor to use the renewable energy, solar light. Silicon-based solar cell has one of critical disadvantage: long-term energy payback time. Fortunately, so far, modern industrial process has reduced its energy payback time to ~ 2 years, but it is necessary to reduce the energy payback time more significantly. However, unfortunately, high-energy required processes are still being used to make photosensitizers for the solar cells, such as II-IV, III-V, I-III-VI semiconductors, quantum dots (QD, synthesized through hot-injection process), polymers, and so on. To reduce the energy payback time significantly, instead of high-temperature and inert gas based synthetic procedure, we propose brand new strategy: perovskite quantum dot synthesis at room temperature in ambient condition. Through in-situ and ex-situ spectroscopic tools, we proposed the formation mechanism of the QDs made through new synthetic process. Furthermore, the intrinsic problem of perovskite – instability against to humidity/water – has been solved by coating silica. We observed the perovskite QDs@SiO_x is stable in water during several weeks.

Poster Presentation : **PHYS.P-248**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Hybrid Composite Ni_xFe_y Alloy and BiVO₄ Photoanode for CO₂ Activation and Reduction in Photoelectrochemical System

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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 for photoelectrochemical (PEC) catalyst of the cathode for the CO₂ reduction reaction. The (040)-BiVO₄ facet engineered photoanode has shown the successful result to improve charge carrier mobility and high photocatalytic active sites for solar light energy conversion. In the photoelectrochemical system, BiVO₄ has been used as a photoanode material which has a function to produce many electrons and protons by the water-splitting reaction. In this study, a hybrid composite cathode using Ni_xFe_y alloy as the pristine base catalyst of the cathode has been used to fabricate the hybrid composite cathode as Nafion/Ppy/rGO/Ni_xFe_y for the CO₂ activation and reduction. The coating of reduced graphene oxide (rGO) and polypyrrole (PPy) layer on the cathode surface with homogeneous and even thin thickness can have each function to increase charge capacity and to activate CO₂ molecule in a reactant state, respectively. CO₂ activation results in lowering the thermodynamic potential energy of the transition state to decrease activation energy of the rate-determining first electron transfer reaction. At the same time, it decreases CO₂ reduction energy. Nafion has also been used to increase the proton conductivity to transport proton into the CO₂ reduction site of the cathode. This system is expected to produce liquid fuel products with high solar to fuel efficiency in the PEC reaction.

Poster Presentation : **PHYS.P-249**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Intramolecular symmetry-breaking charge transfer dynamics of silole-carboranes in solution by femtosecond time-resolved fluorescence

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Icosahedral carborane is a new electron capturing compound with robust stability, and it has been widely investigated as opto-electronic devices. Recently, a silole-carborane compound in which two ortho-carboranes are directly linked to the silole backbone with a phenyl linker has been proposed. Here, we employed a femtosecond fluorescence upconversion technique with about 100 fs time resolution to probe ultrafast population relaxation and charge separation dynamics of silole-carborane compounds in solution. In the femtosecond time-resolved fluorescence, nuclear wavepacket oscillations were resolved in locally excited state, but those were diminished during subsequent charge transfer process. Spectral analysis for time-resolved emission spectra revealed that the charge transfer is solely dependent on polar solvation, and for para-substituted compound, a symmetry-breaking reaction can be occurred exclusively. Quantum calculations supports the asymmetric shift of charge migrations.

Poster Presentation : **PHYS.P-250**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

The effects of cholesterol's preference toward saturated lipid domains on the spatial arrangement and the diffusion of cholesterol in ternary component lipid membranes

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The diffusion of cholesterol in cell membrane is essential to cellular signal transduction such as the formation of cholesterol-enriched domains. The cholesterol diffusion changes with compositions of lipids and the concentration of cholesterol (x_{chol}) in lipid membranes. For example, the presence of unsaturated lipids can significantly facilitate the flip-flop. Also, at high x_{chol} (>0.3) in saturated lipid membrane, cholesterol at the center presents. Since cholesterol at the center is much faster than within leaflets, two diffusivities clearly appear. In multi-component lipid membrane, recent study claimed that cholesterol prefers to locate in saturated lipid domains. However, the diffusion and the spatial arrangement of cholesterol in the system remain elusive at a molecular level. In this study, we perform molecular dynamics simulations for ternary lipid membrane which contains saturated lipids(DPPC), unsaturated lipids(DIPC) and cholesterol to investigate the effects of the cholesterol's preference toward saturated lipid on the spatial arrangement and the dynamics of cholesterol. We find that local x_{chol} in DPPC regions is at least 1.3-fold higher than overall x_{chol} . Therefore two diffusivities clearly appears even at relatively low x_{chol} (~ 0.2). We also compare each pure lipid regions in ternary membrane with comparable binary lipid membranes. The center ratio of cholesterol in DPPC regions ternary membrane is higher than in DPPC binary membrane, which induces more flip-flop in DPPC regions ternary membrane. On the other hand, the center ratio of cholesterol in DIPC regions ternary membrane is lower than in DIPC binary membrane, which induces less flip-flop in DIPC regions ternary membrane.

Poster Presentation : **PHYS.P-251**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

CsPbBr₃@SiO_x Quantum Dot Synthesis under Ambient Condition: Role of Shell for Formation of the Core-shell Structure

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Department of Chemistry, Yeungnam University, Korea

Recent energy demands for human being have raised exponentially. The researches have been dedicated to retarding the global warming by developing the utilization of the alternative energy resources. One of promising renewable energy, solar energy, have been utilized through silicon-based solar cells, which are available in commercial market. However, even though the significant mass production of the Si-solar cells from China have contributed to reduce the energy payback time, however, the Si-solar cell still requires the energy payback time about 2 years. This is because one of the fabrication processes requires the high energy input to melt silicon and generate polycrystalline Si wafer. Compared to the high energy input process, we demonstrated room-temperature synthetic procedure under ambient condition. Fabrication of perovskite quantum dots (PQDs) under ambient condition at room temperature could significantly reduce the energy payback time. We investigated the role of precursors for formation of the core-shell structure, CsPbBr₃@SiO_x. Through in-situ spectroelectrochemical setup, we were able to clarify the formation mechanism of PQD@SiO_x.

Poster Presentation : **PHYS.P-252**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Highly Sensitive Ammonia Gas Sensor Based on Single-crystal Poly(3-hexylthiophene) (P3HT) Organic Field Effect Transistor

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Department of Chemistry, Hanyang University, Korea

We fabricated a Poly-3-hexylthiophene (P3HT) organic single crystal nanowire-based ammonia gas sensor using a LB-nTM transfer method. Our P3HT organic single crystal nanowire – ammonia gas sensor showed higher sensitivity compared to ammonia gas sensor of P3HT organic thin film. The NH₃ concentration range was 0.001ppm to 25ppm at room temperature. The single crystal doesn't have grain boundary and nanowire have a high surface to volume ratio. It is for this reason gas sensing capability of organic single crystal nanowire sensor was demonstrated high sensitivity. In this study, we developed ammonia OFET sensors by employing an array of single crystalline P3HT nanowires as OSC channel and ammonia sensing layer. So we conclude that P3HT single crystal nanowire sensor have high response NH₃ gas and detected lower concentration than P3HT Thin Film sensor.

Poster Presentation : **PHYS.P-253**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Fine-Tuned Charge Carrier Properties of TIPS-Pentacene Single Crystal and its Applications towards Strain Sensing

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High-performance organic electronic devices can be developed by modulating their molecular packing and structures, which typically controls the charge transport properties. In this work, we demonstrate that Monotonic changes in charge carrier mobility of 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-PEN)) from 0.0196 to 19.6 cm²V⁻¹s⁻¹, while subjecting to the wide range of strains from -16.7% (compressive) to 16.7% (tensile). We also found that this massive change in charge carrier mobility in organic single-crystal nanowires due to the change in the intermolecular center-to-center distance by applying uniaxial strain to the cofacially stacked crystals. Finally, we proved these measured values of charge carrier mobility with theoretical calculations based on charge localized hopping theory.

Poster Presentation : **PHYS.P-254**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Study of non-polar Additive Effect on Solvation structure in Lithium-Ion battery electrolytes by FTIR spectroscopy and Internally Referenced DOSY NMR spectroscopy.

Joo Hyun Kim, Chaiho Lim, Kyungwon Kwak*, Minhaeng Cho*

Department of Chemistry, Korea University, Korea

Lithium-Ion batteries are highly demanding battery among other rechargeable batteries due to its high-voltage window and energy density. In the development of lithium-ion batteries, it is important to develop appropriate electrolytes because the electrolyte is a charge carrier in lithium-ion rechargeable battery between anode and cathode material which crucially affects the conductivity of batteries. To understand and enhance the properties of electrolytes, it is important to understand the solvation nature of lithium ion in the electrolytes. Recently, a new method IR-DOSY (Internally Referenced DOSY-NMR) has been reported to study the solvation structure in binary systems that is usually complicated to study in IR spectroscopy. In IR-DOSY, since toluene is not directly participating in the first solvation shell, it is used as an internal reference to calculate the solvation ratio of lithium ions in the electrolyte. So, we research addition of toluene affects the solvation nature of lithium ions in the electrolyte by FTIR spectroscopy. In this study, we represent the effect of toluene to the solvation nature in electrolytes by Fourier-transform infrared spectroscopy (FTIR) and IR-DOSY technique.

Poster Presentation : **PHYS.P-255**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Electrocatalytic Biomass Valorization into Bioplastic Monomer by Transition Metal/Metal Hydroxide Catalysts

Myungjong Kang

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Biomass, which is plant or animal material used as energy source, has been used for entire life of human being. Pristine biomass utilization methods were limited to direct combustion of it or reforming biomass resources to produce biofuels. However, as following the technology advances and demands on utilizing carbon as a resource increases, biomass derived chemicals have been intensively regarded as a new renewable resource. Especially, 5-hydroxymethylfurfural (HMF), produced by dehydration reaction of fructose or glucose, is important platform chemical because it can be converted into 2,5-dimethylfuran (DMF) for biofuel production, adipic acid for nylon synthesis and 2,5-furandicarbaldehyde (DFF) for pharmaceutical. Among those various kinds of HMF-derived chemicals, 2,5-furandicarboxylic acid (FDCA) get attention due to it can replace the petroleum-derived terephthalic acid. By polymerizing FDCA with ethylene glycol, polyethylene furanoate (PEF) is formed, which is good substituent for polyethylene terephthalate (PET). Herein, transition metal/ metal hydroxide based electrocatalyst for HMF oxidation into FDCA is introduced. The introduced electrocatalyst showed 98.5 % of HMF conversion and 96.5 % of FDCA yield, maintaining its catalytic activity after several repeated cycles.

Poster Presentation : **PHYS.P-256**

Physical Chemistry

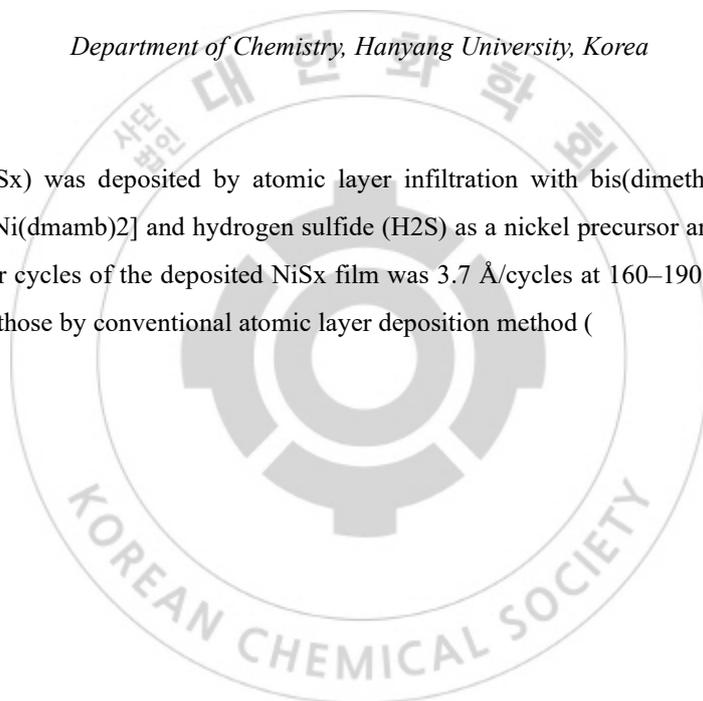
Zoom 6 FRI 16:00~17:00

Rapid growth of Nickel sulfide by atomic layer infiltration and its characterization

Hyeonseok Ji, Myong Mo Sung*

Department of Chemistry, Hanyang University, Korea

Nickel sulfide (NiS_x) was deposited by atomic layer infiltration with bis(dimethylamino-2-methyl-2-butoxo)nickel(II) [Ni(dmamb)₂] and hydrogen sulfide (H₂S) as a nickel precursor and a sulfur precursor. The growth rate per cycles of the deposited NiS_x film was 3.7 Å/cycles at 160–190 °C which was much faster compared to those by conventional atomic layer deposition method (



Poster Presentation : **PHYS.P-257**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Fabrication of large-area single-crystal organic patterned thin films by vertically confined lateral crystal growth

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In this report a one-step fabrication method for large-area single-crystal organic thin films guided through vertically confined lateral crystal growth via capillary force lithography (VC-LCG via CLF) was introduced. We used ink solution of organic molecules that can self-assemble and crystallize within the vertically confined channels of patterned molds. Vertical confinement, determined by the channel depth, played an important role with regard to the crystallization and formation of single-crystalline organic thin films. It was also useful when we fabricated wafer-scale arrays of single-crystal organic thin film transistors, with high performance and uniformly distributed electrical properties, which could be attributed to their large-scale single-crystalline nature, homogeneous film morphologies and the suppression of multiple crystal orientations. In particular, the versatility to various organic molecules, ease of processing optimization, and uniform crystallinity all over the patterned area increase the possibility of VC-LCG to apply in the industrial process.

Poster Presentation : **PHYS.P-258**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

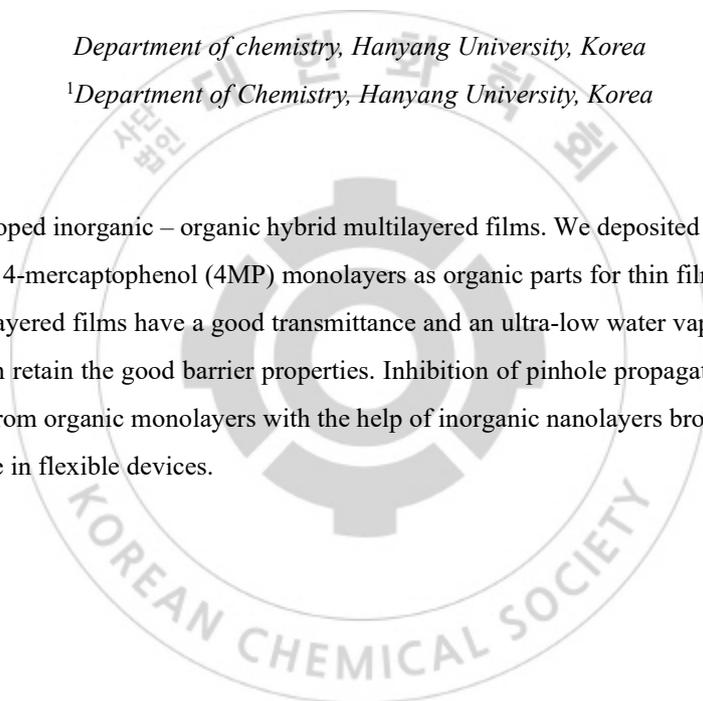
Organic-Inorganic Hybrid Multilayered Films for Encapsulation Layer of Flexible Electronic Devices

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Recently, we developed inorganic – organic hybrid multilayered films. We deposited Al₂O₃ nanolayers as inorganic parts and 4-mercaptophenol (4MP) monolayers as organic parts for thin film encapsulation. The 4MP/Al₂O₃ multilayered films have a good transmittance and an ultra-low water vapor transmission rate. And that films even retain the good barrier properties. Inhibition of pinhole propagation and resistance to mechanical strain from organic monolayers with the help of inorganic nanolayers brought to such superior barrier performance in flexible devices.



Poster Presentation : **PHYS.P-259**

Physical Chemistry

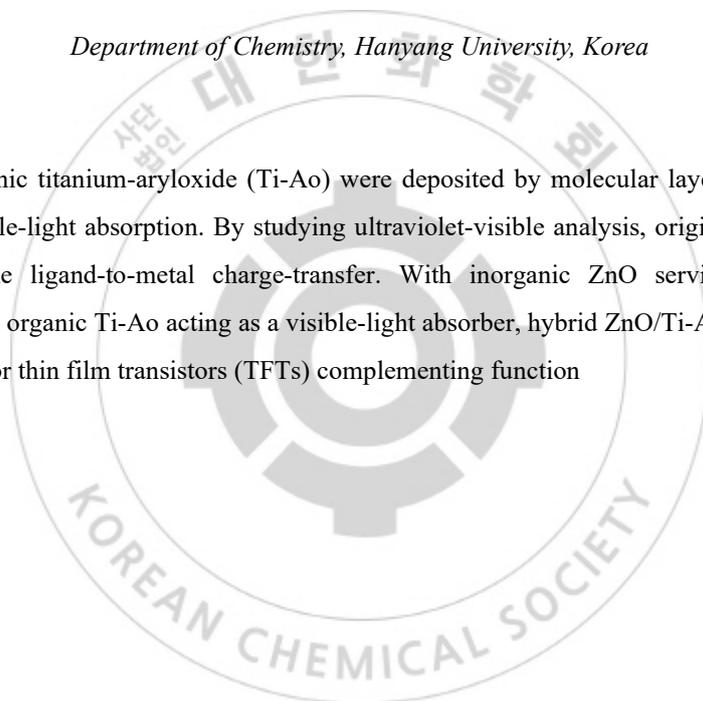
Zoom 6 FRI 16:00~17:00

Hybrid ZnO/Ti-Ao phototransistors with absorption of visible range by using molecular layer deposition

Moohyun Jeong, Myong Mo Sung*

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Thin films of organic titanium-aryloxide (Ti-Ao) were deposited by molecular layer deposition (MLD) showing high visible-light absorption. By studying ultraviolet-visible analysis, origin of the visible light absorption was the ligand-to-metal charge-transfer. With inorganic ZnO serving as an excellent semiconductor, and organic Ti-Ao acting as a visible-light absorber, hybrid ZnO/Ti-Ao thin film was used as active channel for thin film transistors (TFTs) complementing function



Poster Presentation : **PHYS.P-260**

Physical Chemistry

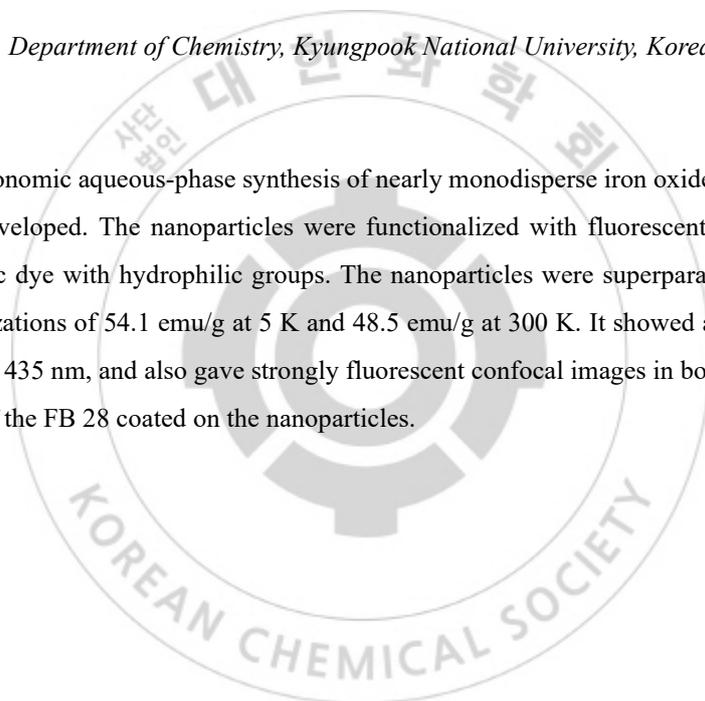
Zoom 6 FRI 16:00~17:00

Magnetic and Fluorescence Properties of Fluorescent Brightener 28-Coated Fe₃O₄ Nanoparticles

Tirusew Tegafaw, Gang Ho Lee*

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In this study, an economic aqueous-phase synthesis of nearly monodisperse iron oxide nanoparticles ($d_{\text{avg}} = 20 \pm 1$ nm) was developed. The nanoparticles were functionalized with fluorescent brightener (FB) 28, which is an organic dye with hydrophilic groups. The nanoparticles were superparamagnetic, with large saturation magnetizations of 54.1 emu/g at 5 K and 48.5 emu/g at 300 K. It showed a strong fluorescence maximum (λ_{max}) at 435 nm, and also gave strongly fluorescent confocal images in both the green and blue regions, because of the FB 28 coated on the nanoparticles.



Poster Presentation : **PHYS.P-261**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Poly(acrylic acid) coated five different ultras-small heavy metal oxide (Bi₂O₃ , Yb₂O₃ , NaTaO₃ , Dy₂O₃ , and Gd₂O₃) nanoparticles as potential CT contrast agents

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Ultras-small heavy metal-oxide nanoparticles can be utilized for highly enhancing contrasts in computed tomography (CT). Their potential as CT contrast agents were investigated by measuring their X-ray attenuation properties for five different polyacrylic acid (PAA)-coated ultras-small heavy metal oxide (Bi₂O₃ , Yb₂O₃ , NaTaO₃ , Dy₂O₃ , and Gd₂O₃) nanoparticles. The estimated average particle diameters for PAA-coated ultras-small nanoparticles by using transmission electron microscopy were (Bi₂O₃ 2.3nm, Yb₂O₃ 1.7nm, NaTaO₃ 1.5nm, Dy₂O₃ 1.8nm, and Gd₂O₃ 1.9nm). The observed X-ray attenuation power was stronger than that of a commercial iodine CT contrast agent (Ultravist®) at the same atomic concentration and much stronger at the same number density, proving the potential of ultras-small nanoparticles for use as a powerful CT contrast agent. The effectiveness of the nanoparticle suspension samples as CT contrast agents was demonstrated by acquiring in vivo CT images by using one of the samples (i.e. PAA-coated ultras-small Bi₂O₃ nanoparticles). After intravenous injection into the mouse-tail vein, positive contrast enhancements in various organs were observed.

Poster Presentation : **PHYS.P-262**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

D-glucosamine conjugated polyacrylic acid (PAA) coating ultrasmall Gd₂O₃ nanoparticles and the effect on the water proton relaxivities of different ligand

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Magnetic resonance imaging has become a powerful tool for diagnosis due to the valuable researches on the MRI contrast agents. For biomedical application MRI-CAs nanoparticle should be stable, highly water soluble, non-toxic, and ultrasmall in particle size. In this work, we used PAA connected with different concentration of D-glucosamine as water soluble and biocompatible ligand for the surface coating of the nanoparticles. They were characterized by HRTEM, XRD, FT-IR, TGA, Cytotoxicity and Map image. The nanoparticles were found monodisperse and average particle diameter is estimated to be ~2 nm. And non-toxic for biomedical application.

Poster Presentation : **PHYS.P-263**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Non-adiabatic Time-Dependent Wave-Packet Study of The Proton-Coupled Electron-Transfer in NH₃Cl complex

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A charge-transfer excited state (CT) of NH₃Cl complex (H₂N⁺-H-Cl⁻) is produced by photo-detachment of an electron from NH₃Cl⁻ anion, which proceeds into two different reaction pathways i.e., NH₂ + HCl (proton transfer; PT) and NH₃ + Cl (electron transfer; ET), corresponding to a typical case of proton-coupled electron transfer (PCET) process. To study the early-time dynamics of this CT, time-dependent wave-packet propagation on non-adiabatically coupled three electronic states within reduced three-dimensional space was performed. The XMS-CASPT2/aug-cc-pVTZ level of theory was applied for evaluating the adiabatic electronic states of neutral NH₃Cl complex. The initial dynamics of PCET process up to about 100 fs was described in detail by using the population dynamics of coupled three electronic stages, while the branching ratio (χ) defined as the ratio of PT to ET, $\chi = \text{PT}/\text{ET}$, was determined after the wave-packet propagation up to 2000 fs. In addition, the dependences of χ on vibration levels of initial precursor anion and isotope substitution of the connecting H with deuterium and tritium were also investigated. Our results revealed the detailed microscopic features of this PCET process as well as systematic dependences of the branching ratio χ on the above factors.

Poster Presentation : **PHYS.P-264**

Physical Chemistry

Zoom 6 FRI 16:00~17:00

Folic Acid-Conjugated Polyacrylic Acid-Coated Ultrasmall Manganese Oxide Nanoparticles : In Vivo Positive Magnetic Resonance Imaging of Brain Cancer

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Ultrasmall nanoparticles are potential candidates for application as high-performance imaging agents. Herein, we present the synthesis and characterization of folic acid (FA)-conjugated polyacrylic acid (PAA)-coated MnO nanoparticles with an average particle diameter of 2.7 nm. FA conferred cancer-targeting ability while PAA conferred good colloidal stability and low cellular cytotoxicity on the FA-PAA-coated MnO nanoparticles. Further, the nanoparticles exhibited a high relaxivity (r_1) value of $9.3 \text{ s}^{-1}\text{mM}^{-1}$ ($r_2/r_1 = 2.2$). Their application potential as cancer-targeting T_1 magnetic resonance imaging contrast agents was confirmed by their enhanced T_1 contrast enhancements at the brain cancer (U87MG) site upon intravenous administration to mice tails.

Poster Presentation : **PHYS.P-265**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Impact of the Dynamic Electron Correlation on the Unusually Long Excited State Lifetime of Thymine

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Non-radiative relaxation of the photoexcited thymine in the gas-phase shows an unusually long excited-state lifetime, previously attributed to trapping in the absorbing excited state (the S₂-trapping). Here, we investigate this mechanism using the non-adiabatic molecular dynamics (NAMD) simulations combined with the recently developed Mixed Reference Spin-Flip Time-Dependent Density-Functional Theory (MRSF-TDDFT) method. We show that the S₂-trapping was an artifact caused by an insufficient account of electron correlation. The current work predicts instead the S₁-trapping mechanism with two lifetimes, $\tau_1=30\pm 1$ fs and $\tau_2=6.1\pm 0.035$ ps, quantitatively consistent with the time-resolved experiments. Upon excitation to the S₂($\pi\pi^*$) state, thymine undergoes an ultrafast (ca.30 fs) S₂ \rightarrow S₁ internal conversion and resides around the minimum on the S₁($n\pi^*$) surface slowly decaying to the ground state (ca.6.1 ps). While the S₂ \rightarrow S₁ internal conversion is mediated by fast bond length alternation distortion, the subsequent S₁ \rightarrow S₀ occurs through several conical intersections involving a slow puckering motion.

Poster Presentation : **PHYS.P-266**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Ultrasmall Gadolinium Oxides Nanoparticles as Multifunctional Agent: MRI, Tumor Detection and Gadolinium Neutron Capture Therapy

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Magnetic resonance imaging (MRI) is widely used as noninvasively diagnostic tool because MRI has high spatial resolution and high sensitivity. Besides, MRI could combine with a therapeutic agent, in which one compound is able for both diagnosis and therapy of diseases. From that perspective, gadolinium nanoparticles have great potential to work as theragnostic agents. First of all, gadolinium ion (Gd(III)) has seven unpaired 4f electrons ($8S7/2$), which give large electron magnetic moment, and besides, Gd(III) also induce efficiently the longitudinal relaxation of water protons, making Gd(III) ion the most suitable T1 MRI contrast agent. Another point should be taken into consideration is that gadolinium has high thermal neutron capture cross-section (σ), for example ^{157}Gd isotope has σ value of 254000 barns, that is 60 times larger than the σ value of ^{10}B , a commonly used agent for boron neutron capture therapy (BNCT). Therefore, gadolinium nanoparticles are promising candidates for neutron capture therapy of tumors. Herein, poly(acrylic acid)-rhodamine coated gadolinium oxide nanoparticles were synthesized and used as MRI, tumor detection agent and in vitro gadolinium neutron capture therapy agent (GdNCT) of human glioblastoma astrocytoma (U87MG) cells.

Poster Presentation : **PHYS.P-267**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Polyacrylic Acid-coated Terbium(III) and Holmium(III) Oxide Nanoparticles : Synthesis, Characterizations, and 9.4 Tesla T₂ MR Images

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

Polyacrylic acid (PAA)-coated lanthanide oxide (Ln₂O₃) nanoparticles (NPs) (Ln = Tb and Ho) with high colloidal stability and good biocompatibility were synthesized, characterized, and investigated as a new class of negative (T₂) magnetic resonance imaging (MRI) contrast agents at high MR fields. Their r₂ values were appreciable at 3.0 T MR field and higher at 9.4 T MR field whereas their r₁ values were negligible at all MR fields, indicating their exclusive induction of T₂ relaxations with negligible T₁ relaxation inductions. Their effectiveness as T₂ MRI contrast agents at high MR fields was confirmed from strong negative contrast enhancements in in vivo T₂ MR images at 9.4 T MR field after intravenous administration into mice tails.

Poster Presentation : **PHYS.P-268**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids

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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-269**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Cost-efficient, Effect of Low-Quality PbI₂ Purification to Enhance Performances of Perovskite Quantum Dots and Perovskite Solar Cells

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Yeungnam University, Korea

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In modern society, high-quality material development and a large stable supply are key to perform frontier research and development. However, there are negative issues to address to utilize high-quality resources with a large stable supply for research, such as economic accessibility, commercialization, and so on. One of the cutting-edge research fields, perovskite-related research, usually requires high-quality chemicals with outstanding purity (>99%). We developed an economically feasible PbI₂ precursor with around 1/20 cost-down for perovskite/perovskite quantum dots through recrystallization and/or hydrothermal purification. Following the methodology, the quantum dots from both as-prepared and purified PbI₂ demonstrated identical photophysical properties, with a photoluminescence quantum yield (PLQY) of 52.61% using the purified PbI₂ vs. 45.83% PLQY using commercial PbI₂. The role of hydrothermal energy was also checked against the problematic PbI₂, and we checked whether the hydrothermal energy could contribute to the hindrance of undesired particle formation in the precursor solution, which enables them to form enlarged grain size from 179 ± 80 to 255 ± 130 nm for higher photoconversion efficiency of perovskite solar cells from 14.77 ± 1.82% to 15.18 ± 1.92%.

Poster Presentation : **PHYS.P-270**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Photo-induced twisting dynamics of photo-sensitizing D- π -A organic dyes in film by picosecond time-resolved fluorescence

HyunJae Lee, Jeongmin Ji¹, Hwan Kyu Kim, Chul Hoon Kim*

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The donor- π -bridge-acceptor (D- π -A) architecture of a metal-free organic dye has been well established in the field of dye-sensitized solar cell (DSSC). In this study, three new D- π -A-structured organic sensitizers, named as SGT-138, 150 and 151, has been synthesized and their photo-physical properties were fully investigated in film by picosecond time-resolved fluorescence spectroscopy. In the previous study, it was revealed that the DSSCs with the SGT dyes with CDCA and HC-A1 co-adsorbents exhibit good power conversion efficiencies, but their electron injection efficiencies are determined to be unexpectedly low because a fast deactivation process in locally excited state, which is comparable to the charge injection rate, was always resolved even in the film with a large excess of the co-adsorbents. To unveil the fast non-radiative processes, time-resolved emission spectra (TRES) of the dyes anchored on Al₂O₃ and TiO₂ surfaces were directly recorded in the full spectral range. We found that a photo-induced structural distortion is responsible for such the fast reaction, and that is sensitive to the bridge structure as well as the type of co-adsorbent.

Poster Presentation : **PHYS.P-271**

Physical Chemistry

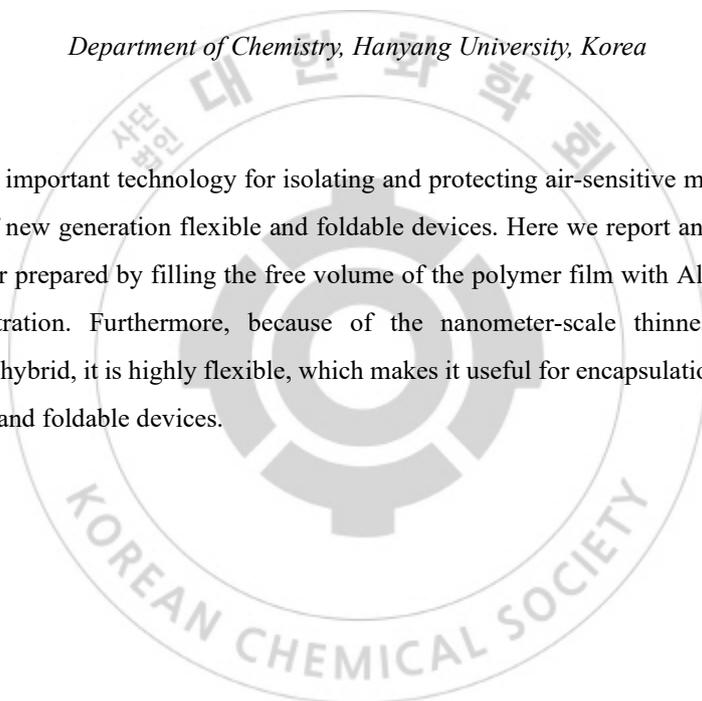
Zoom 7 FRI 15:00~16:00

Ultra Gas-Proof polymer for devices using by Atomic Layer Infiltration

Jaeyoung Park, Hongrho Yoon, Myong Mo Sung*

Department of Chemistry, Hanyang University, Korea

Encapsulation is an important technology for isolating and protecting air-sensitive materials and is key in the development of new generation flexible and foldable devices. Here we report an extremely enhanced gas diffusion barrier prepared by filling the free volume of the polymer film with Al₂O₃ using gas-phase atomic layer infiltration. Furthermore, because of the nanometer-scale thinness of the complete polymer-inorganic hybrid, it is highly flexible, which makes it useful for encapsulation technology of new generation flexible and foldable devices.



Poster Presentation : **PHYS.P-272**

Physical Chemistry

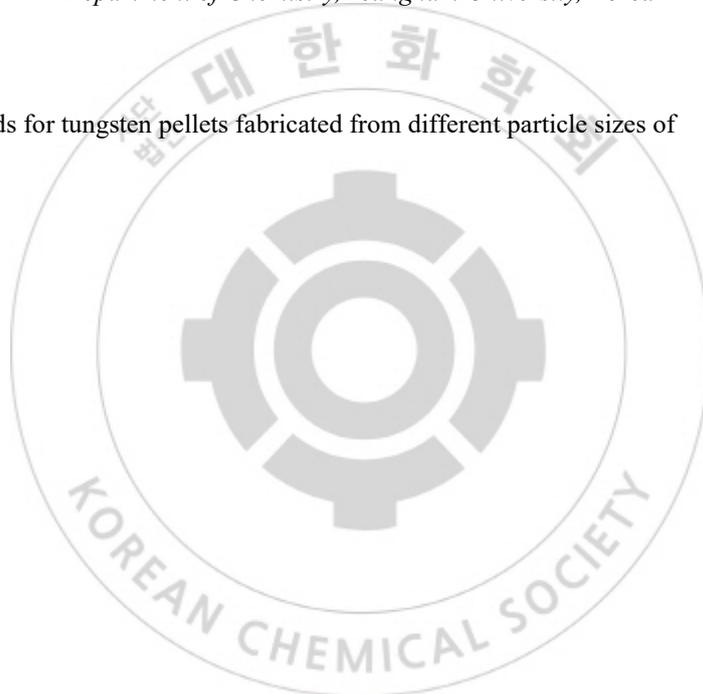
Zoom 7 FRI 15:00~16:00

Change in the sputtering yield of tungsten by pre-heating treatment

JeongWoo Nam, Young-Sang Youn*

Department of Chemistry, Yeungnam University, Korea

The sputtering yields for tungsten pellets fabricated from different particle sizes of



Poster Presentation : **PHYS.P-273**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Study on the lattice thermal expansion for zirconium samples containing minor alloying elements

Jeong Min Ha, Young-Sang Youn*

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The change in the lattice parameter of zirconium samples containing minor alloying elements of tin, niobium, iron, and chromium as well as the simulated ZIRLO and Zircaloy-4 samples in the temperature range of 30-870 °C was studied by *in situ* high-temperature X-ray diffraction (HT-XRD). Through Pawley refinement of *in situ* HT-XRD spectra, we confirmed that the *a* -axis lattice parameters of zirconium samples added with niobium, iron, and chromium for the hexagonal Zr crystal structure were larger than the lattice constant obtained from a zirconium sample due to the lattice thermal expansion at all temperatures. On the other hand, the *a* -axis lattice constant of zirconium sample with tin was smaller than that of the zirconium sample. In addition, the *c* -axis lattice parameters for all zirconium samples containing minor alloying elements were mostly greater than those of zirconium sample. Furthermore, in simulated ZIRLO and Zircaloy-4 samples, the lattice parameters of the *a* -axis were smaller than those of a zirconium sample, whereas the *c* -axis lattice parameters were larger than those of a zirconium sample.

Poster Presentation : **PHYS.P-274**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Mechanism of the Photoinduced Ring-Opening Reaction in Dihydroazulene

Svetlana Shostak, Cheol Ho Choi*

Department of Chemistry, Kyungpook National University, Korea

The energy consumption is increasing early. Currently, gas and coal 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, photochromic molecules (especially photoswitches) 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-vinylheptafulvene. Severe geometric difference between the initial compound and the one formed as the result of photoexcitation makes this molecule a particularly attractive subject to study. 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 reaction. Several conical intersections involved in the reaction were obtained, and their role in the deexcitation process was shown via NAMD calculations. The quantum yield of several products was calculated based on the NAMD outcome as well. Additionally, low quantum yield hydrogen transfer in DHA was shown for the first time.

Poster Presentation : **PHYS.P-275**

Physical Chemistry

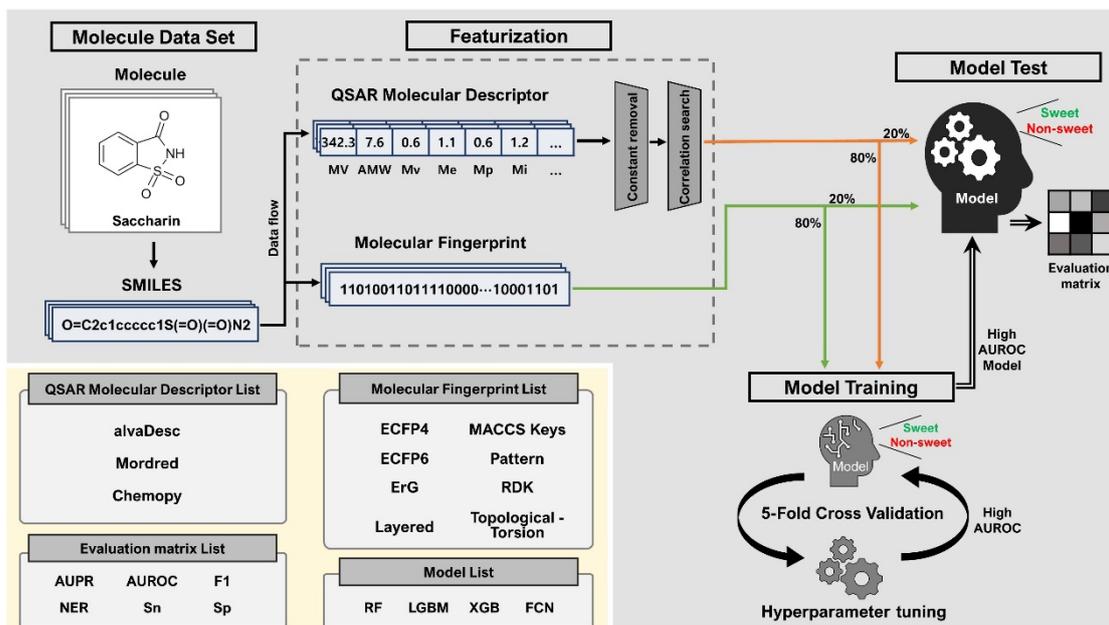
Zoom 7 FRI 15:00~16:00

Sweetness property prediction and molecule structure analysis with machine learning

Junho Lee, Seon Bin Song, You Kyoung Chung, Joonsuk Huh*

Department of Chemistry, Sungkyunkwan University, Korea

The desire for healthy life of the public and the ever increasing consumption of the sweeteners make the researchers intent to non-nutritive sweetener in spite of some development difficulty such as high development cost and poor knowledge for sweetness molecules. With this present condition, the research and development necessity of sweetness molecules is obvious. Recently, machine learning studies for sweetness prediction have been steadily reported to help the development of new sweetness molecules. However, the most of studies have focused on reporting the high performance of machine learning models while a few studies have reported the lack of feature analysis. In this point of view, we suggest the improved prediction model and the advanced feature analysis for sweetness molecules. Our machine learning model, Light Gradient Boosting Machine, (LGBM) has high performance scores with AUROC 0.946 for alvaDesc molecular descriptor features and AUROC 0.955 for layered fingerprint features. We find that the molecules which have many high substituted amines are impossible to have sweetness by the feature analysis. In addition, based on the ligand binding approach, the sweetness molecules need hydrogen bond donor sites. It is also important that the topology of atoms, geometry of chemical active site, and the existence of specific substructures of molecule. Our study can provide the development efficiency in time and cost, because it gives the guideline to the sweetness molecule design and prediction model as pre-test method for new theoretically designed sweetness molecules. Therefore, we suggest that which properties of the molecules affect the sweetness prediction by features analysis of the high scored machine learning model with a chemical perspective.



Poster Presentation : **PHYS.P-276**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Photoinduced acid-base reaction in AOT reverse micelles

Hak-won Nho, Oh-Hoon Kwon*

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Reverse micellar (RM) systems are the simplest experimental systems mimicking water pockets in biology to uncover the reaction in biologically relevant environment. The RM system consists of a hydrophobic phase outside, a hydrophilic surface structure toward inside core region and polar substance confined by the surface. When the polar solvent is water, the core is usually considered into two portions as bound and free water region. The hydrophilic layer strongly binds the water molecules resided on this portion. It makes less polar and rigid structure of bound water molecules than distal free water. This structural feature induces a confined heterogenic environment with dielectric and viscosity gradients in the nanopool core. We have introduced a unique prototropic probe, N-methyl-7-hydroxyquinolinium in the AOT RM to investigate how hydration dynamics and excited-state proton-transfer (ESPT) reaction of the prototropic charged probe responds to the confined and heterogeneous of environment [1,2]. After the photoexcitation, deprotonation of excited-state cationic species (C*) gives rise to a neutral keto species (K*) as the product. The strong ionic interaction between anionic surface of RM and the probe diminishes during ESPT. It leads migration of C* toward the core region of RM after ESPT. This ESPT-assisted diffusion was verified by monitoring time-resolved fluorescence decay of each species. The emission bands originated from these two species in the time-resolved emission spectra were deconvoluted by fitting them with lognormal band shape functions. By following the time-dependent changes of peak intensity and Stokes shift for each deconvoluted band, we separately verified the residence site of two species in the RM structure and the kinetics of the ESPT. Reference[1]A. Adhikari, J.-H. Park, H.-W. Nho and O.-H. Kwon, *J. Mol. Liq.* 2020, 320, 114346.[2]H.-W. Nho, J.-H. Park, A. Adhikari and O.-H. Kwon, *J. Mol. Liq.* 2021, 326, 115270.

Poster Presentation : **PHYS.P-277**

Physical Chemistry

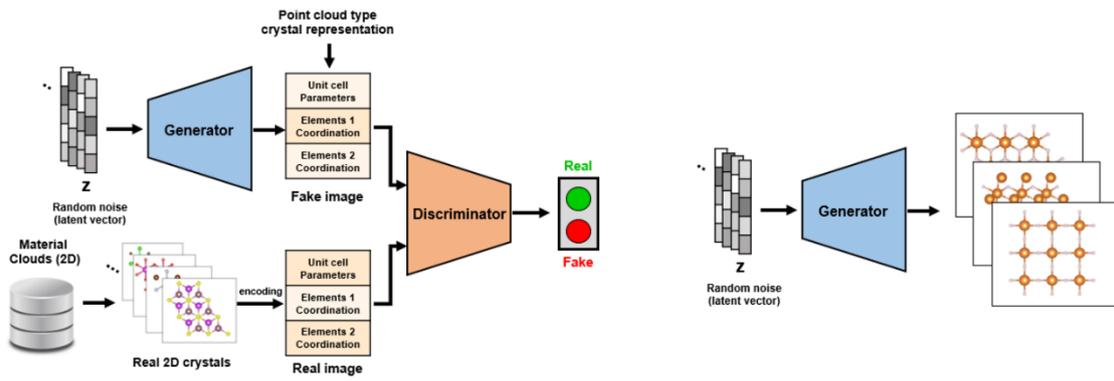
Zoom 7 FRI 15:00~16:00

Theoretical identification of 2D monolayer MgH₂ for hydrogen storage materials

Junho Lee, Joonsuk Huh*

Department of Chemistry, Sungkyunkwan University, Korea

Hydrogen energy, a promising clean energy that can be utilized as a promising energy carrier in 21st century, has recently been actively studied in a wide range of applications. However, there is still a difficult problem in designing new hydrogen storage materials with high gravimetric density. Two-dimensional metal hydride (2D MH), the chemical hydrogen host material with a large hydrogen capacity and surface area, is likely to be used as a thermal stable and low-cost hydrogen storage material. In recent years, studies on extensive structural explorations in 2D MH have been conducted and about 100 stable 2D MH have been reported through substitution-based material prediction method. In this work, we report a novel structure of 2D magnesium hydride (MgH) through systematic theoretical study using deep learning-based generative models and density functional theory (DFT). We find that P-4m2 MgH₂ is thermodynamic stable and a good candidate for hydrogen storage materials. Furthermore, structures that allow Li atoms to be doped onto the surface to adsorb additional multiple hydrogen molecules also investigated. Therefore, a theoretical foundation is provided for the applications of multiple-phase 2D MgH₂ was provided in hydrogen storage domains that combine artificial intelligence (AI) and DFT calculations.



Learning 2D crystal structures

Generating unknown phase 2D MgH_2



Poster Presentation : **PHYS.P-278**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

multi-layer Nafion/PVP/rGO/NiFe-LDH/Cu system for efficient and selective photoelectrochemical CO₂ reduction

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Sogang University, Korea

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Carbon dioxide (CO₂) is one of the reasons for global warming and climate change. Hence, CO₂ reduction and converting it into useful products is an important issue in day today life. There are different methods used to reduce and convert CO₂ into useful products such as high-pressure temperature, electrochemical, photochemical and photoelectrochemical methods etc. However, all these methods have individual plus and minus points, among them low efficiency is a most critical and vital point need to be overcome. The one reason behind low efficiency is its highly stable and linear structure, which provides low absorptions and slow reactivity. Moreover, CO₂ reduction into useful products is a multi-step process; it requires multiple electrons and protons for useful products such as methanol. By considering all these points, herein multi-layer electrode as Nafion/PVP/rGO/NiFe-LDH/Cu has investigated for efficient and selective CO₂ reduction by photoelectrochemical way. A NiFe-LDH will be useful for high capacitance and conductivity, rGO will be responsible for multi electron shuttling that would be helpful for the product selectivity, PVP's N-site can act as adsorption and activation of CO₂ molecule and as Nafion is well-known as proton transfer material so it can increase the proton diffusion rate and overall reaction will be accelerated in efficient way. A NiFe-LDH layer was confirmed by XRD, thickness of each layer was observed by SEM. Electrochemical properties of each layer were studied and investigated by LSV, CV and EIS.

Poster Presentation : **PHYS.P-279**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Characterization of PEG-*b*-PNiPAAM Hydrogel Drug the Heating and Cooling Process

Minkyong Kim, Yeonju Park¹, Young Mee Jung*

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¹*Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*

Thermoresponsive polymer, poly(*N*-isopropylacrylamide) (PNiPAAM) has phase transitions at specific temperature which is lower critical solution temperature (LCST). PNiPAAM has been widely used in drug delivery systems because its LCST is similar to physiological body temperature. However, PNiPAAM has a risk for accumulating in the body. To overcome this problem, PNiPAAM has been copolymerized with poly(ethylene glycol) (PEG), which is biodegradable polymer. In this study, the temperature-dependent IR spectra are analyzed using principal component analysis (PCA) and two-dimensional correlation spectroscopy (2D-COS), to investigate PEG-*b*-PNiPAAM hydrogel the thermal behavior of PEG-*b*-PNiPAAM. Results will be discussed in this presentation.

Poster Presentation : **PHYS.P-280**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Detection of Neurotoxic Pesticides Using Surface-enhanced Raman Scattering

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²*Division of science education, Kangwon National University, Korea*

It is important to detect neurotoxic pesticides which have caused long-term harm to people, quickly and sensitively. In this study, we detected neurotoxic pesticides based on surface-enhanced Raman scattering (SERS) using tyramine signal amplification (TSA). By using the TSA method, a lot of hotspots were generated, and the enhanced factor was increased by 3.58 orders compared to conventional SERS. As a result, the limit of detection of thiabendazole as one of neurotoxic pesticides was 0.1 μM . Details of the results will be discussed in the presentation.

Poster Presentation : **PHYS.P-281**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

The effects of various force fields on the properties of organic ionic plastic crystals

Seewoo Park, Bong June Sung^{1,*}

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¹*Department of Chemistry, Sogang University, Korea*

It is of importance to employ appropriate force fields when trying to simulate molecular systems. Especially when one aims to simulate charged systems such as ionic liquids, not only electrostatic interactions between charges but also the polarizability affects various physical properties. In this work, we investigate how different types of force fields lead to different static and dynamic properties for a representative case of organic ionic plastic crystals (OIPCs). OIPCs are a novel class of materials composed of molecular ions and may undergo rotational relaxations in solid crystal phases. Such active rotational motion of ions allows dopants (such as lithium ions) to diffuse readily even in solid phases. Therefore, OIPCs have been considered as a strong candidate for the solid electrolytes of all solid-state batteries. We perform atomistic molecular dynamics simulations of 1-methyl-3-methylimidazolium hexafluorophosphate ([MMIM][PF₆]) at temperatures from 75 to 500K under isothermal-isobaric conditions (NPT), and consider four kinds of force fields: (1) CL&P, (2) OPLS, (3) Atomistic Polarizable Potential for Liquids, Electrolytes, & Polymers (APPLE&P), (4) nonpolarizable versions of APPLE&P. While APPLE&P takes the polarizability into account, other do not. APPLE&P provides the density (1.7 g/cm³ at 175K), which is consistent well with experiments (1.698 g/cm³ at 173K). Simulations with all the four force fields show that rotational relaxations of ions in crystals can be activated depending on temperature but the rotational dynamics is spatially heterogeneous. The polarizable force field APPLE&P, however, predicts a much faster rotational relaxation, which will certainly affect the diffusion and the conductivity of lithium ions.

Poster Presentation : **PHYS.P-282**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Au Decorated Fe₃O₄@TiO₂ Nanoparticles as a Vis Region Active Photocatalyst

Sila Jin, Yeonju Park¹, Young Mee Jung*

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¹*Kangwon Radiation Convergence Research Support Center, Kangwon National University, Korea*

Most organic dyes are highly stable and have a very long residence time in the water, which makes serious water pollution. In the last few decades, catalysts for quickly and simply decomposing organic dyes have been developed. TiO₂ is a promising material in photocatalytic research due to its low toxicity, stability, and high reactivity. However, because of the large bandgap energy and high recombination rate, pure TiO₂ is limited as a photocatalyst. In this study, by decorating Au nanoparticles (Au NPs) on the TiO₂ surface, Au NPs decorated Fe₃O₄@TiO₂ nanocomposites were fabricated which not only acts as an electron acceptor but also reduces bandgap energy, enabling catalytic activity in the visible region. Details on its characterization and analysis will be discussed in this presentation.

Poster Presentation : **PHYS.P-283**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

The cooling rate effects of the mechanical properties of glassy polymer fibers

Taejin Kwon, Bong June Sung*

Department of Chemistry, Sogang University, Korea

Polymer glasses are out of equilibrium and thus their properties depend on the thermal history like the cooling rate. For example, many studies showed that the glass transition temperature increases with increasing the cooling rate. The mechanical properties of polymer glasses would be also affected by the cooling rate. However, the cooling rate effects on the mechanical properties of polymer glasses are yet to be understood at a molecular level. In this work, we perform molecular dynamics simulations for polymer melts by employing a coarse-grained bead spring model. We investigate the stress-strain curves of polymer glasses. We show that the value of yield stress increases with decreasing the cooling rate, which is the same with the experimental results of typical polymer glasses. We also investigate the local stress and local elastic modulus of polymer glasses. We find that the cooling rate affects the spatial distribution of local modulus. In the more slowly cooled glasses, the spatial distribution of local elastic modulus is much broader. We show that the fluctuation of the local stress of polymer glasses is a key factor to understand the cooling rate effect on the mechanical properties of polymer glasses.

Poster Presentation : **PHYS.P-284**

Physical Chemistry

Zoom 7 FRI 15:00~16:00

Structure-Mediated Interface Effects and Charge Transfer on SERS Activity of MoS₂-Ag-rGO

Shuang Guo, Lei Chen¹, Sila Jin, Eungyeong Park², Young Mee Jung*

Department of Chemistry, Kangwon National University, Korea

¹College of chemistry, Jilin Normal University, China

²Kangwon National University, Korea

Semiconductor materials were widely used in the process of SERS detection due to their unique physical and chemical properties. Especially the interface effects of semiconductors in composite structures can effectively increase the charge transfer effect in complex system. To study this effect, we adopt a simple hydrothermal method to prepare the 2D+2D MoS₂-Ag-rGO composite structure and precisely control reaction temperature to realize the regulation of contact interface. Comparing the SERS spectra between this composite structure and simple MoS₂ nanospheres, we explore the relationship between SERS signal and contact interface of material and charge transfer mode. We further verified this relationship by using intrinsic Raman and XPS spectra. The details of the relationship between SERS effect and semiconductor interface will be discussed in this presentation.

Poster Presentation : **PHYS.P-285**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Thermal fluctuation of magnetic weight of the Ag/Fe₃O₄ ferromagnetic nanoparticle assembly

Hackjin Kim

Department of Chemistry, Chungnam National University, Korea

The magnetic nanoparticles greater than the critical size show the ferromagnetic behaviors and assemble rapidly when placed under the magnetic field. The magnetic weight of the ferromagnetic nanoparticle sample, that is, the magnetic force experienced by the magnetic nanoparticles under the magnetic field increases as the nanoparticles assemble to form a regular lattice. We have observed the thermal fluctuation of the magnetic weight of the Ag/Fe₃O₄ ferromagnetic nanoparticle sample under the magnetic field. The lattice structure of the assembled nanoparticles is perturbed by the thermal motions of the nanoparticles. The magnetic weight of the nanoparticle sample decreases with the temperature rise, and vice versa. This characteristics of the ferromagnetic nanoparticles suggests that the ferromagnetic nanoparticles could be used as a magnetic thermometer.

Poster Presentation : **PHYS.P-286**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Core-shell silica coated Fe₃O₄ Nanobeads as adsorbents for Magnetic Separation of Nucleic Acids

Huan Yue, Gang Ho Lee^{1,*}

Department of Chemistry, Kyungpook National University, China

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

Recently, a lot of researches on magnetic nanobeads which have attracted extensive attentions, because of their strong superparamagnetic properties and specific binding properties of the surface functional groups, they can be applied to the separation of biological molecules such as nucleic acids, DNA, RNA and proteins from blood samples. In this study, the separation of nucleic acids from blood samples of patients was studied. To this end, core-shell structured silica coated iron oxide (SiO₂@ Fe₃O₄) nanobeads were synthesized Stöber method, and characterized by X-ray diffraction (XRD), Fourier transformed-infrared spectroscopy (FT-IR), high-resolution transmission electron microscopy (FE-TEM), and vibrating sample magnetometry (VSM). The synthesized SiO₂@ Fe₃O₄ nanobeads exhibit a size distribution of 40-50 nm and a shell thickness is around 10nm. In addition, in vitro cytotoxicity showed a good biocompatibility. They showed excellent adsorption and magnetic separation performance for the purification of nucleic acids from patients' blood samples. Therefore, the SiO₂@ Fe₃O₄ nanobeads showed the successful magnetic separation performance.

Poster Presentation : **PHYS.P-287**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Control of intersystem crossing dynamics of blue-phosphorescent Ir(III) complexes probed by time-resolved luminescence

HyungJoo Lee, Ho-Jin Son, Sang Ook Kang, Chul Hoon Kim*

Department of Advanced Materials Chemistry, Korea University, Korea

Blue phosphorescent organometallic materials with Iridium metal center have been getting extensive attention in the field of OLEDs because of their high emission efficiency. However, it is well known that their intrinsic photolysis process in higher excited state can deteriorate the performance of OLED device, but its origin is not well established yet. Here, we prepared a series of blue phosphorescent Ir(III) complexes with varying ligand structures and electron withdrawing group, and fully investigated their photo-physical properties by excitation dependent quantum yield and time-resolved optical spectroscopic measurements. We found that the intersystem crossing (ISC) of the Ir(III) complex with a tert-phenyl ligand was highly decelerated without any ultrafast component, and it was sensitive to the position of HOMO levels (the effect of the electron withdrawing group). Quantum calculations revealed that the frontier orbital (LUMO) for singlet MLCT (metal-to-ligand charge transfer) state is fully localized at the tert-phenyl moiety that is perpendicularly linked to the main backbone, but that for triplet state is rather shifted to the metallic center. This indicates that weak electronic coupling between singlet and triplet states causes such the slow ISC.

Poster Presentation : **PHYS.P-288**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

ZnO composite nanolayer showing mobility edge quantization for developing multi-value logic transistors

Jongchan Kim, Myong Mo Sung*

Department of Chemistry, Hanyang University, Korea

A unique composite nanolayer material based on ZnO which contains quantized conducting states has studied. It was applied to develop multi-value logic transistors with an intermediate state other than ON and OFF in binary systems. A composite nanolayer that embeds ZnO quantum dots in an amorphous ZnO matrix generated a quantized conducting state at the mobility edge, and the phenomenon was referred to as “mobility edge quantization”. As the emergent states are quantized and possess a minimal density of states, the gate-bias independent charge density in the composite nanolayer enables a current saturation. The multi-value logic transistors were based on the hybrid superlattice which consists of alternating composite ZnO nanolayers and organic layers. The superlattice channel exhibited multiple states due to the current saturation in the composite nanolayers. Our multi-value transistors showed superb performances such as stable and reliable operation without current fluctuation, and controllable multi-level states (e.g., binary, ternary, and quaternary) by changing the number of the ZnO layers.

Poster Presentation : **PHYS.P-289**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Excited-state Intramolecular Charge Transfer Dynamics of Aminoanthraquinones in Confined Environments of Reverse Micelles

Taehyung Jang, Gisang Lee, Yoonsoo Pang*

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

Photo-induced intramolecular charge transfer (ICT) of chromophores have been of great interest in chemistry and biology fields for the applications to solar energy conversion, photovoltaics, and fluorescence sensing. 1-Aminoanthraquinone (AAQ) shows ultrafast (150-180 fs) ICT dynamics in the excited state with the rotation of the amino (-NH₂) group attached to the anthraquinone backbone. In our recent femtosecond stimulated Raman spectroscopy (FSRS) measurements, the major vibration modes including $\nu_{C-N} + \delta_{CH}$ (1200-1230 cm⁻¹) and $\nu_{C=O}$ (1300-1330 cm⁻¹) of AAQ showed the ICT dynamics and strongly couplings to the low frequency deformation modes including the intermolecular hydrogen bond network with solvent dimethyl sulfoxide molecules. In this research, the excited-state dynamics of 1-AAQ and its structural isomer, 2-aminoanthraquinone in the confined environment of reverse micelles are investigated by time-resolved electronic and vibrational spectroscopy. Since solvents confined in the nanopools of the reverse micelles show distinct solvent properties from bulk such as decreased solvation dynamics or largely increased viscosity, the ICT dynamics of AAQs accompanied with the rotation of the amino group are expected strongly perturbed in the reverse micelle environments. The photophysical properties of AAQs in the reverse micelles will also be investigated by varying the local environments such as the micelle size or surfactant charges.

Poster Presentation : **PHYS.P-290**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Structural changes of “push-pull” dyes during the intramolecular charge transfer

Sebok Lee, Myungsam Jen, Yoonsoo Pang*

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

The Intramolecular charge transfer (ICT) between the electron donor and acceptor is considered as one of the fundamental chemical reactions, and of great interest in chemistry and related fields. The ICT of "push-pull" dyes have been widely investigated by many time-resolved spectroscopy, where the electron donor and acceptor groups are connected by or bond. Many theoretical studies often suggest the structural changes of the chromophore upon the ICT either in the molecular geometry of the electron donor or acceptor groups. However, such structural changes with the ICT were not clearly observed from many experimental studies. Recently, we reported the ICT of 4-dicyanomethylene-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran (DCM) by femtosecond stimulated Raman spectroscopy (FSRS), where a twisted structure with the rotation of the electron donating dimethylamino group was suggested from the Raman spectral and simulation results from time-dependent density functional theory (TDDFT) method. In this work, similar "push-pull" dyes with the electron acceptor nitro group, 4-dimethylamino-4'-nitrobiphenyl (DNBP) and 4-dimethylamino-4'-nitrostilbene (DNS), have been investigated by FSRS with both high spectral (ν) and temporal (τ) resolution. Upon excitation, abrupt changes of these modes were observed mainly in the frequency region of 1550-1650 cm^{-1} , where twisting of the biphenyl group with ultrafast ICT dynamics of 300-500 fs was suggested for the structural changes during the ICT process. The TDDFT simulations also support the twisted geometries of the nitrophenyl group for the ICT states of DNBP and DNS in the excited states. Lastly, the current developments in impulsive stimulated Raman spectroscopy setup for the investigation of low-frequency skeletal vibrational modes and solute-solvent interaction modes will also be briefly introduced.

Poster Presentation : **PHYS.P-291**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Metal-Enhanced Fluorescence by the Quadrupole Surface Plasmon Resonance of Silver Nanoparticles

Daedu Lee, GyoungHyun Song, Yoonsoo Pang*

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

Metal-enhanced fluorescence (MEF) has been widely studied for wide applications including biological imaging, chemical sensing, and organic optoelectronics due to the improved molecular brightness and photostability. MEF results from the increased local electric field and the plasmon-coupled emission, which accompanies the through-space energy transfer between dyes and surface plasmon resonance (SPR). The dipole SPR modes of gold or silver nanoparticles have been predominantly adopted in most MEF studies since the properties of dipole SPR can be controlled rather simply by changing the size and shape of nanoparticles. On the other hand, MEF by the quadrupole SPR has been reported by several recent studies, where the detailed emission kinetics including the plasmon-coupled emission and the energy transfer between dyes and the quadrupole SPR were not investigated. In this work, fluorescence enhancement and kinetics of dyes will be studied with homogeneous silver colloidal films (SCFs) composed of silver spherical nanoparticles of 60-220 nm diameter. The SCFs with larger nanoparticles than ~100 nm diameter show the strong quadrupole SPR modes with a similar wavelength dependence on the size of silver nanoparticles as the dipole SPR. The fluorescence of dyes were strongly enhanced with the decrease in lifetime when the significant spectral overlap occurs between the emission bands of dyes and the dipole or quadrupole SPR bands of SCFs, which denotes that the quadrupole SPR modes can be similarly adopted in many MEF applications as the dipole SPR modes.

Poster Presentation : **PHYS.P-292**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

DFT Study on Hydrogen Evolution Reaction on Fe and P doped WS₂ surface

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

With the goal of the development of non-noble efficient catalysts for the water splitting, we studied iron and phosphorus doped tungsten sulfide (Fe/P-WS₂) as a promising catalyst for hydrogen evolution reaction (HER). The Fe/P-WS₂ surface phenomena were investigated with density functional theory (DFT) calculations. The theoretically examined catalyst delivered superior activity, conductivity, and appropriate Gibbs free energy change (ΔG_H) towards HER, also the simulated crystal parameters with GGA-PBE and Grimme's DFT-D3 functional were well consistent with as obtained experimental results.

Poster Presentation : **PHYS.P-293**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Electron Push–Pull Effects on Intramolecular Charge Transfer in Perylene-Based Donor–Acceptor Compounds

Mina Ahn, Kyung-Ryang Wee*

Department of Applied Chemistry, Daegu University, Korea

A series of asymmetric donor–acceptor (D–A) perylene-based compounds, 3-(N,N-bis(4'-(R)-phenyl)amino)perylene (**Peri-DPA(R)**) were successfully prepared to explore their intramolecular charge transfer (ICT) properties. To induce ICT between donor and acceptor, diphenylamine (DPA) derivatives (electron donor units) with same functional groups (**R**= CN, F, H, Me, or OMe) at both para positions were linked to the C-3 position of perylene to produce five **Peri-DPA** derivatives. A steady-state spectroscopy study on **Peri-DPA(R)**s exhibited a progressively regulated ICT trend consistent with the substituent effect as it progresses from the electron withdrawing group to the electron donating group. In particular, a comparative study using a D–A–D (donor–acceptor–donor) system demonstrated that not only electron push-pull substituent effect but also subunit combinations influence photophysical and electrochemical properties. Observed different ICT characters in Lippert-Mataga plots of **D–A(CN)** and **D–A–D(CN)** (CN-substituted **D–A** and **D–A–D**), led to the investigation on whether ICT emission of two systems with differences in subunit combinations is of the same type or different type. Femtosecond transient absorption (fs-TA) spectroscopic results provided direct evidence of ICT origin and confirmed that **D–A(CN)** and **D–A–D(CN)** exhibited the same transition mix of ICT (from donor to acceptor) and reverse ICT (rICT, from arylamine to CN unit). DFT/TD-DFT calculations support the presence of ICT for all five compounds and the experimental observations of rICT presented only for CN-substituted compounds.

Poster Presentation : **PHYS.P-294**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

SERS Investigation of Gold Nanoparticles Encapsulated High Plasma Treated Paper Substrate for Environmental Pollutant monitoring

Rashida Akter, Suyeon Hong¹, Ilsun Yoon^{2,*}

Department of chemistry, Chungnam National University, Korea

¹*Chemistry, Chungnam National University, Korea*

²*Department of Chemistry, Chungnam National University, Korea*

We developed a paper based gold nanoparticles (AuNPs) plasmonic substrate where the AuNPs were grown by the plasma-reduction of pre deposited Au ions onto high plasma treated cellulose filter paper. AuNPs of nm gaps are formed with high surface coverage on the fiber surfaces by optimizing the plasma power and treatment time. The AuNPs encapsulated high plasma treated cellulose substrate shows strongly enhanced SERS activities of benzenethiol (BT) with the enhancement factor (EF) of 1.5×10^7 with a relative standard deviation (RSD) of 3.4 %. The enhanced SERS sensitivities of these AuNPs paper substrates are evaluated by applying the substrates for ultrasensitive detection of malachite green in deionized (DI) water. The results show that the proposed paper-based SERS substrate could selectively and reproducibly detect 1 fM in DI water. The proposed AuNPs paper SERS substrates would have the advantages of simplicity in the preparation and ultrasensitive detection of environmental pollutants.

Poster Presentation : **PHYS.P-295**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Excited state intramolecular proton transfer dynamics studied by stimulated Stokes and anti-Stokes Raman spectroscopy

Myungsam Jen, Sebok Lee, Gisang Lee, Yoonsoo Pang*

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

Proton transfer reaction is one of fundamental chemical reactions and of great interest in chemistry and biology disciplines. Excited state intramolecular proton transfer (ESIPT) occurring on ultrafast time scales have been investigated in many femtosecond spectroscopic methods. We have reported the ESIPT of 1,2-dihydroxyanthraquinone (alizarin) by femtosecond stimulated Raman spectroscopy (FSRS), where the proton transfer from a hydroxyl to the adjacent carbonyl groups occurs with a time constant of 110 fs in dimethyl sulfoxide (DMSO). The solvent DMSO also plays an important role in the ESIPT of alizarin. The solvent vibrational modes of DMSO, (S=O) and (CSC) showed ultrafast spectral changes especially in the “free” and “aggregated” subbands during the ESIPT of alizarin, which is interpreted as the consequence of the intermolecular hydrogen bonding between alizarin and surrounding DMSO molecules. In this work, FSRS measurements in the Stokes (Raman gain type) and anti-Stokes (Raman loss type) frequencies will be introduced to explain further details of the ESIPT and solvent dynamics of alizarin in DMSO. By observing the vibrational modes of DMSO in both Stokes and anti-Stokes regions, we hope to be able to differentiate changes resulting from the solvation processes and thermal effects. The (CH) mode of DMSO can also be observed with anti-Stokes measurements, which may provide important kinetic information for the solvation dynamics during and after the ESIPT of alizarin.

Poster Presentation : **PHYS.P-296**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Artificial cell models with enhanced physical and mechanical properties

Huong Thanh Nguyen, Sungwoo Jeong¹, Kwanwoo Shin^{2,*}

Chemistry, Sogang University, Vietnam

¹*Research Institute for Basic Science, Sogang University, Korea*

²*Department of Chemistry, Sogang University, Korea*

One of the grand challenges in synthetic biology is to fabricate the artificial cell membrane with enhanced the physical and mechanical properties. The membrane is required to be stable against the changes in the surrounding microenvironments which are required for the incorporation of various reactions inside. However, current cell membrane models including lipid bilayer and vesicles hardly reflect the crowded conditions of plasma membrane. Here, we developed protein crowding giant lipid vesicles by integrating extracellular matrix proteins to narrow the gaps between artificial and plasma membranes. This enhanced stability of the membrane will facilitate the investigation of cellular activities in a simplified and isolated in vitro environment of artificial cell.

Poster Presentation : **PHYS.P-297**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

A Facile Synthesis Method and Excited-State Dynamic of the highly ordered Poly(3-hexylthiophene) Crystalline particles

Seung Jin Jung, Jaehong Park^{1,*}

Chemistry & Nanoscience, Ewha Womans University, Korea

¹*Department of Chemistry and Nanoscience, Ewha Womans University, Korea*

Regioregular Poly(3-hexylthiophene) (rr-P3HT) used in organic photoelectric applications has different photoelectronic properties depending on its morphology such as crystalline or amorphous structures. These morphological features therefore impact on the device performance. Thus, in order to understand the exact photoelectronic properties of crystalline P3HT only, we fabricated highly crystalline P3HT particles (P3HT-CPs). P3HT crystalline-particles (P3HT-CPs) were prepared by an antisolvent slow-diffusion method. These P3HT-CPs feature pre-deposition condensed phase structures with particle dimensions spanning from 100s nm to micron size scale. XRD and TEM characterization results of the P3HT-CPs suggest well-ordered packing between polymer backbones along the (100) direction and substantially suppressed polymer amorphous fractions. Excited-state dynamics was studied with amorphous P3HT particles. In contrast to transient absorption spectroscopic signatures in structurally heterogeneous rr-P3HT, these P3HT-CPs lacks spectral shift, demonstrating homogeneous P3HT packing. These microscopic and optical spectroscopic results indicate that P3HT-CPs is well made without amorphous structures through an antisolvent slow-diffusion method, and P3HT-CPs is a special model system that can study the exact exciton dynamics in crystalline polymers.

Poster Presentation : **PHYS.P-298**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Transformation of optical properties and crystal phase in self-doped Ag₂Se nanocrystals

Kwang Seob Jeong^{*}, Haemin Song

Department of Chemistry, Korea University, Korea

Localized Surface Plasmon Resonance(LSPR) in a semiconductor has been of great interest for recent years since it is expected to retain a unique property that combines the quantized energy and LSPR, which are the characteristics of semiconductor and metal, respectively. Here, we present the appearance of LSPR starting from intraband in self-doped Ag₂Se nanocrystals. By fitting the experimental data to the k.p model and the Lorentzian functions, we proved that LSPR property gradually mixed with the excitonic transition as the nanocrystal size increases. The photoluminescence, the unique character of excitonic transition, also demonstrated the emergence of LSPR property by an attenuated intraband PL intensity. Interestingly, the peak splitting resulted from the nondegenerate 1Pe state was observed with increasing LSPR character, which simultaneously happens with the crystal phase transformation from cubic to tetragonal. The observed transformation from intraband to LSPR with crystal phase change has potential to pave the way for the new colloidal quantum to plasmon hybrid optoelectronics and provides an opportunity to consider the effect of crystal phase on carrier density.

Poster Presentation : **PHYS.P-299**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

The Grunwald-Winstein Relationship of 2-Methyl-2-Adamantyl Chloroformate under Solvolytic Conditions

Seoyeon Jang, Jieun Lee¹, Kyoung-Ho Park^{2,*}, Hoshik Won³, Jin Burm Kyong^{3,*}

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In hydroxylic solvents, the solvolysis of 2-methyl-2-adamantyl chloroformate was studied at various temperatures. The sensitivities to changes in nucleophilicity and solvent ionizing power of the extended Grunwald-Winstein equation ($\log (k/k_0) = lN_T + mY_{Cl} + c$) are calculated from the rate constants. These values were similar to those for solvolyses of 1-adamantyl chloroformate over the full range of solvents, suggesting that the unimolecular mechanism involving the step of ion pairs is rate-determining. This aspect was also compared with those reported for the corresponding 2-adamantyl and alkyl haloformates, previously.

Poster Presentation : **PHYS.P-300**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

In Vitro Cytotoxicity, and Relaxometric Properties of Water-Soluble Chitosan Oligosaccharide Lactate-Coated Gadolinium Oxide Nanoparticles

Mohammad Yaseen Ahmad, Gang Ho Lee^{1,*}

Department of Chemistry, Kyungpook National University, India

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

In this study, the suitability of Chitosan oligosaccharide lactate (COL) as a surface-coating material of gadolinium oxide NPs is explored. COL-coated ultrasmall gadolinium oxide NPs were synthesized through a one-pot polyol method. The synthesized COL-coated gadolinium oxide NPs were subject to various analyses to measure their particle diameter, hydrodynamic diameter, crystal structure, and surface coating. Furthermore, in vitro cellular cytotoxicity was measured to evaluate their biocompatibility. Water proton spin relaxivities and map images were also measured to evaluate their potential as a T₁ MRI contrast agent.

Poster Presentation : **PHYS.P-301**

Physical Chemistry

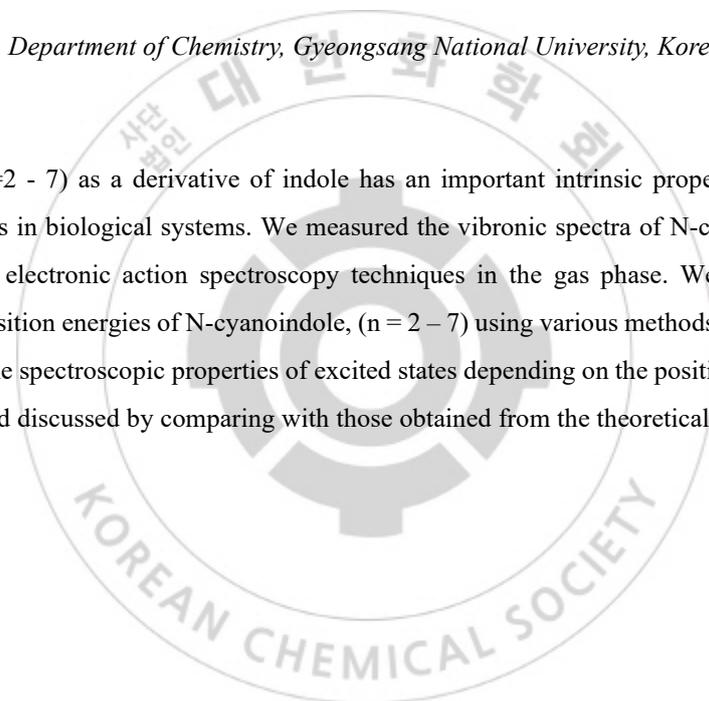
Zoom 7 FRI 16:00~17:00

Laser Spectroscopy and Quantum Chemical Calculation of an Indole derivatives: a Position-dependent study

Juhyeon Park, Ahreum Min, Cheol Joo Moon, Jiwon Kim, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

N-cyanoindole ($n=2 - 7$) as a derivative of indole has an important intrinsic property for its enormous biological activities in biological systems. We measured the vibronic spectra of N-cyanoindole ($n=2 - 7$) monomer through electronic action spectroscopy techniques in the gas phase. We also calculated the ionization and transition energies of N-cyanoindole, ($n = 2 - 7$) using various methods (DFT and TD-DFT) with a basis set. The spectroscopic properties of excited states depending on the position of the $C\equiv N$ group are investigated and discussed by comparing with those obtained from the theoretical calculations.



Poster Presentation : **PHYS.P-302**

Physical Chemistry

Zoom 7 FRI 16:00~17:00

Improved Double-Hybrid Density Functional with Restricted Open-Shell Hartree-Fock Orbitals

Hayoung Yu, Suhwan Song, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

Open-shell systems are essential in many reactions of chemical interest, such as transition states in reaction barrier heights, reagents for bond formation and breaking, and reactions including transition metal complexes. For decades, the unrestricted (U) scheme has been widely used to handle open-shell configurations. Combining this with the Kohn-Sham density functional theory (KS-DFT) indeed explains the electronic structure well. For Hartree-Fock (HF), however, unphysical phenomena such as spin-contamination cause non-negligible errors in radical systems. Thus, using the HF orbitals as a reference to the post-HF methods or the HF-DFT approaches sometimes gives inaccurate results. In this presentation, we address such difficulties and limitations of the UHF scheme. We also apply a restricted open-shell HF (ROHF) scheme to BL1p, a recent double-hybrid functional [J. Phys. Chem. Lett. 12, 800 (2021)], and the results are compared with the U scheme.

Poster Presentation : **PHYS.P-303**

Physical Chemistry

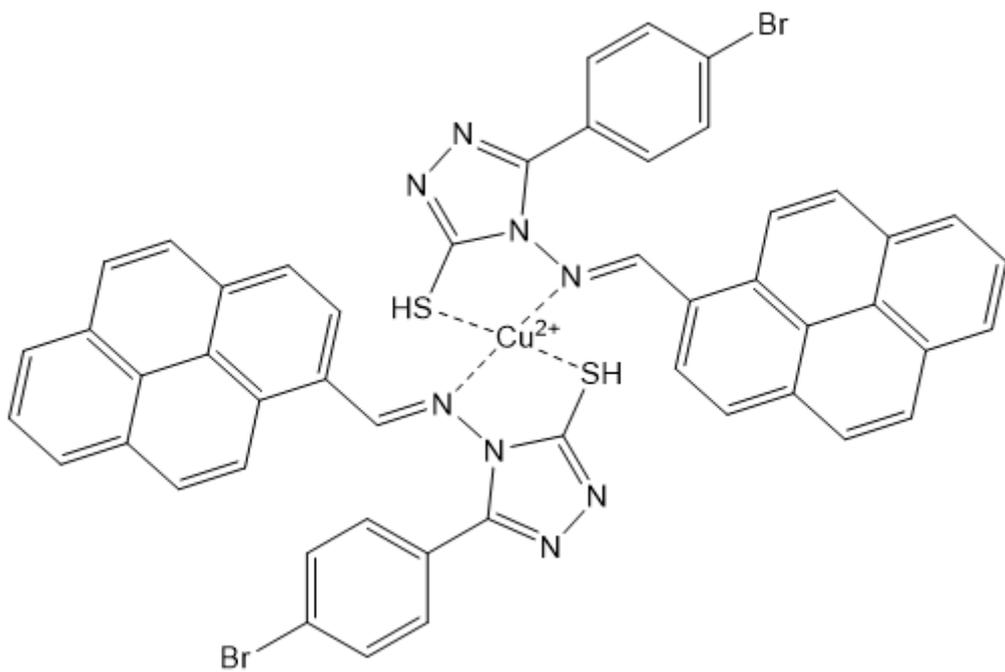
Zoom 7 FRI 16:00~17:00

Schiff base functionalized 1,2,4-Triazole and Pyrene derivatives for selective and sensitive detection of Cu²⁺ in the aqueous medium

Nam Gyu Choi, Hyang-Im Ryoo, Ki Hwan Lee*

Department of Chemistry, Kongju National University, Korea

We have prepared Schiff base functionalized 1,2,4-Triazole and Pyrene derivatives for selective, sensitive, and naked eye colorimetric detection of Cu²⁺ in the aqueous medium. Amongst the 19 different metal ions studied for absorption and fluorescence titration, only Cu²⁺ ion induces the change in color and spectral properties of Schiff base functionalized 1,2,4-Triazole and Pyrene probe. The stoichiometric ratio of the probe-Cu²⁺ complex was determined to be 2:1 according to Job's plot. The lower detection limit estimated for Cu²⁺ is 0.234nM which shows excellent sensitivity and selectivity of the present analytical method towards detection of Cu²⁺ ion in the aqueous medium. The present approach has been successfully utilized for the quantitative determination of Cu²⁺ ion from environmental aqueous solution.



Poster Presentation : **PHYS.P-304**

Physical Chemistry

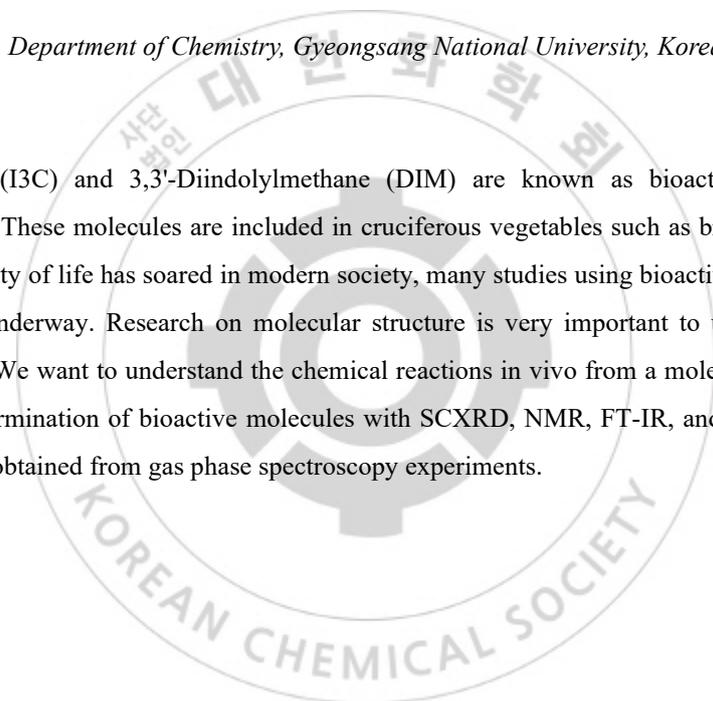
Zoom 8 FRI 15:00~16:00

Structural Analysis of I3C and DIM Using the Gas-Phase Laser Spectroscopy and Computational Chemistry

Jiwon Kim, Ahreum Min, Cheol Joo Moon, Juhyeon Park, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Indole-3-carbinol (I3C) and 3,3'-Diindolylmethane (DIM) are known as bioactive molecules with anticancer effects. These molecules are included in cruciferous vegetables such as broccoli and cabbage. As interest in quality of life has soared in modern society, many studies using bioactive molecules as well as medicine are underway. Research on molecular structure is very important to understand chemical reactions in vivo. We want to understand the chemical reactions in vivo from a molecular perspective by analyzing the determination of bioactive molecules with SCXRD, NMR, FT-IR, and UV-VIS compared with the structure obtained from gas phase spectroscopy experiments.



Poster Presentation : **PHYS.P-305**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Chiral Metasurface from Two Thumbs

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¹Chemistry, Chungnam National University, Korea

Biological structures inspired metasurface design and fabrication accord unique surface functionalities. Human fingerprint is one of the fascinating 2-dimensional bio-surface that possesses complex surface pattern. Here, human fingerprint - mimetic 3-dimensional elastomeric grating meta-skin (EGMS) is fabricated by adopting its surface curvature. The EGMS metasurface was composed of a series of isochronal pattern on flexible polymer film. It was able to tune its chiral properties through the control of the direction of surface pattern (aka., blaze arrow, A) and tangent vector (T) to induce symmetry breaking. That is, its chirality is readily tuned to be left- and right-handed by modulating the skew angle (\square) between two operators. From these experiments of EGMS, the origin of chirality in human fingerprint was observed and introduced a facile method to impart tunable chiroptical properties on the metasurfaces, which may probably extend essential insights for chiral thin film structure for metasurface research.

Poster Presentation : **PHYS.P-306**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Second-Harmonic Generation Phase of Hetero-Bilayer TMDs

Juseung Oh, Sunmin Ryu*

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

Two-dimensional (2D) materials have recently gained much research interest for their novel properties and potential applications. Optical second-harmonic generation (SHG) has become important methodology for characterizing 2D materials. SHG is a non-linear optical process in which a non-centrosymmetric optical medium interacts with two photons and generates a photon with a doubled frequency. Whereas SHG intensity has found immediate application in imaging crystalline domains and orientations of 2D materials, SHG phase has rarely been studied despite its potential of discovering new phenomenon. In this work, we present a progress in modeling and measuring SHG phase of monolayer and hetero-bilayer TMDs. Compared to monolayer TMDs, hetero-bilayers are predicted to exhibit more complex phase behavior because of interlayer optical interference as their crystal orientation is varied. Moreover, an additional degree of freedom in hetero-bilayers, adjustable stacking angle, will allow modulation of SHG phase and ultimately contribute to custom-tailored non-linear light conversion. We will also discuss preliminary SHG phase data obtained by interferometric detection with a confocal laser scanning microscope.

Poster Presentation : **PHYS.P-307**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

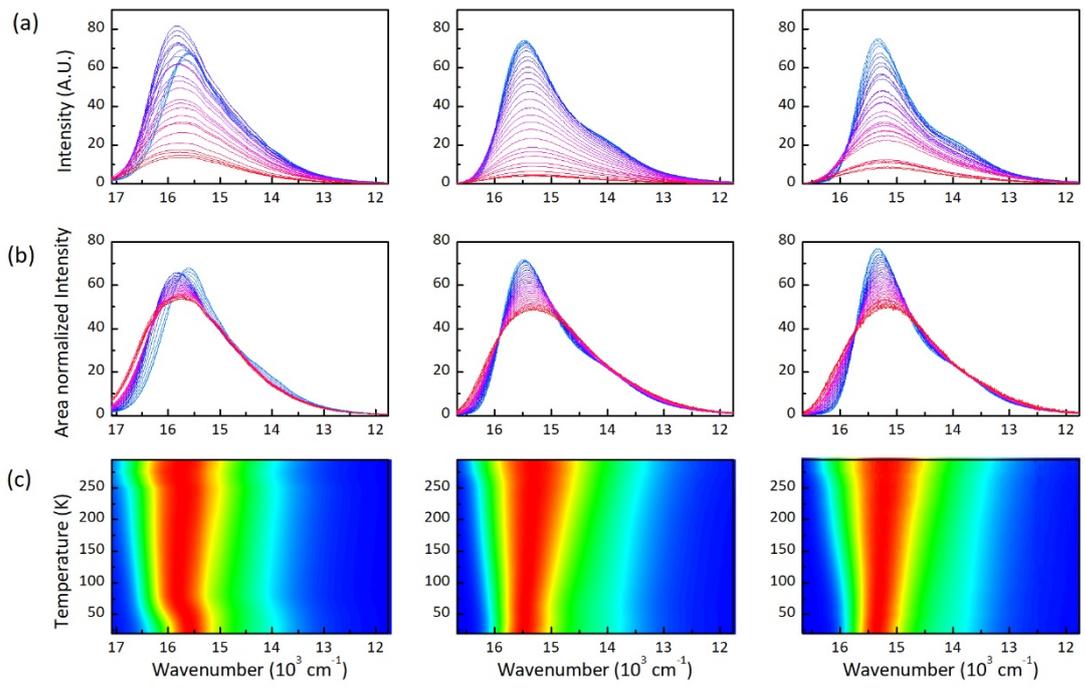
The Study on Structural Characteristics of Red Fluorescence Protein (RFP) at Cryogenic Temperature for Improvement of RFP Performance

Taecheon Lyu, Taiha Joo^{1,*}

Chemistry, Pohang University of Science and Technology, Korea

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

RFPs are advantageous for use as fluorescent probes of living animal cell owing to their properties, such as reduced autofluorescence, low light scattering, and low absorbance at longer imaging wavelengths. In this study, the frequency- and time-resolved spectroscopy at cryogenic temperatures were performed for the RFPs using a closed-cycle helium (He) cryostat. We observed the changes of structure and optical properties owing to the volume contraction and the Boltzmann distribution at low temperatures. By directly investigating the excited state of the RFPs, we attempted to determine which structural characteristics contribute to the improvement of RFP performance, including brightness. The figure shows the stationary fluorescence spectra of mKate (left), mNeptune1 (middle), and mCardinal2 (right) at varying temperature 20–295 K (blue–red lines). The spectral change below the freezing point, that is, the jagged change of mKate and consistent blue shift of mNeptune and mCardinal, is related to the structural rearrangement by the volume reduction at low temperatures. For mKate, the contracted volume after freezing increases the planarity of the twisted phenol ring of the chromophore, which leads to a red shift in the emission spectrum up to 240 K. Below 240 K, the spectrum shifts toward blue again owing to the misalignment by excessive contraction. On the other hand, the phenol rings of mNeptune and mCardinal were originally flat because of the Ser158Cys mutation, thus the flatness is broken in the reduced cavity at low temperatures. The clear isoemissive point of the temperature-dependent area-normalized emission spectra support the coexistence of flat and twisted conformers at low temperatures.



Poster Presentation : **PHYS.P-308**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Photoexcitation dynamics of $[\text{CpFe}(\text{CO})_2]_2$ in solution

Jisik Jung, JuHyang Shin, Manho Lim*

Department of Chemistry, Pusan National University, Korea

Photochemistry of $[\text{CpFe}(\text{CO})_2]_2$ known as a typical metal carbonyl complex has been investigated broadly but details of the reaction mechanism is far from established. Femtosecond time-resolved IR spectroscopy of $[\text{CpFe}(\text{CO})_2]_2$ can reveal molecular structures of nascent products, reaction intermediates, and products of the photoreaction. Time-resolved IR spectra will be obtained in broad time range after excitation of $[\text{CpFe}(\text{CO})_2]_2$ in various solvent with 340 nm pulse. Photoexcitation of $[\text{CpFe}(\text{CO})_2]_2$ is known to produce $\text{CpFe}(\text{CO})_2$ radical and $\text{CpFe}(\mu\text{-CO})_3\text{CpFe}$, which can react with halocarbon solvent (CCl_4 and CHCl_3) producing $\text{CpFe}(\text{CO})_2\text{Cl}$. Details of solvent-dependent photoreaction of $[\text{CpFe}(\text{CO})_2]_2$ and bimolecular reaction with chlorocarbon solvent will be presented.

Poster Presentation : **PHYS.P-309**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

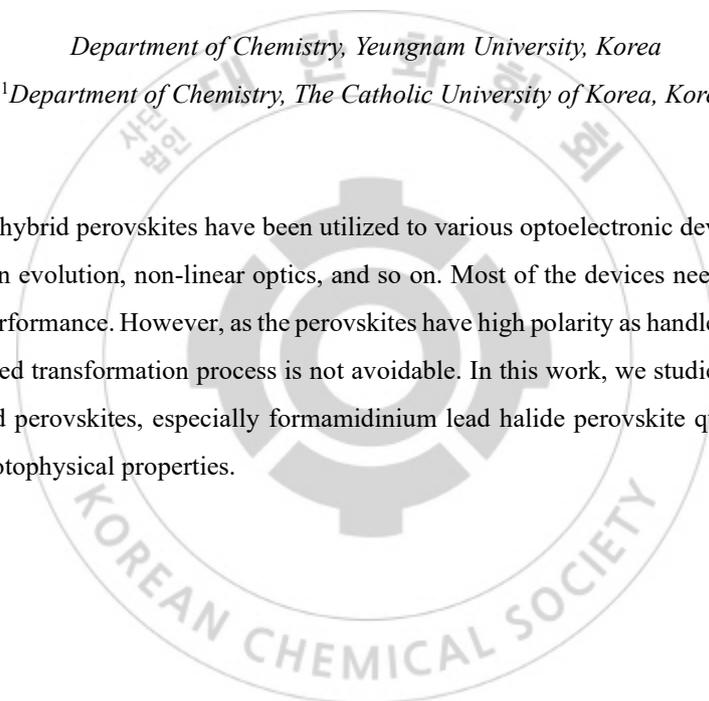
Role of Electric Field for Formamidinium Lead Halide Perovskite Quantum Dots

YeJi Shin, ChaeHyun Lee, Kyoungsoo Kim¹, Donghoon Han^{1,*}, Seog Joon Yoon^{*}

Department of Chemistry, Yeungnam University, Korea

¹Department of Chemistry, The Catholic University of Korea, Korea

Organic-inorganic hybrid perovskites have been utilized to various optoelectronic devices such as display, solar cell, hydrogen evolution, non-linear optics, and so on. Most of the devices needs to apply electrical field to test their performance. However, as the perovskites have high polarity as handled to “soft materials”, electric field induced transformation process is not avoidable. In this work, we studied the role of electric field for the hybrid perovskites, especially formamidinium lead halide perovskite quantum dots, to their modulations of photophysical properties.



Poster Presentation : **PHYS.P-310**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Laser Assisted Green Synthesis of Lignin Mediated gold Nanoparticles in Aqueous Media

**Hyecheon Lee, Yewon O¹, Shreyanka Shankar Naik, Yiseul Yu, Seung Jun Lee¹, Myong
Yong Choi^{1,*}**

Chemistry, Gyeongsang National University, Korea

¹Department of Chemistry, Gyeongsang National University, Korea

The development of an eco-friendly and reliable process for the production of nanomaterials is essential to overcome the toxicity and exorbitant cost of conventional methods. This is produced by reducing Au precursors using lignin biopolymers which are formulated by second harmonic pulsed laser irradiation and an ultrasonication process. Lignin containing functional groups, which operates as both a reducing and stabilizing agent. The various analytical techniques of UV-visible, FE-TEM, XRD studies were employed to verify the formation of L-Au NPs. The optimized lignin-Au NPs composite was investigated for the detection of toxic heavy metal of Pb⁺ ions (1mM) in an aqueous environment. Hence, the cost effectiveness, stability and environmental friendliness of L-Au NPs make it a promising functional material for removing lead from wastewater.

Poster Presentation : **PHYS.P-311**

Physical Chemistry

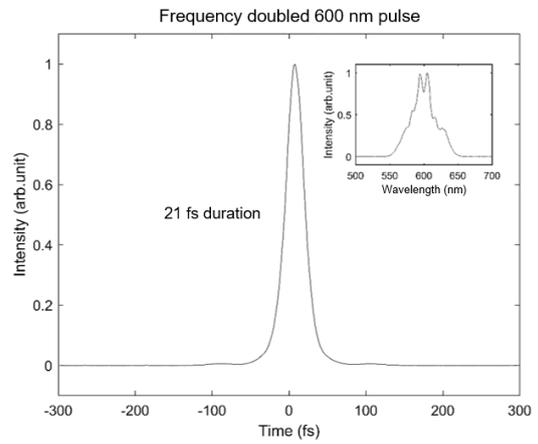
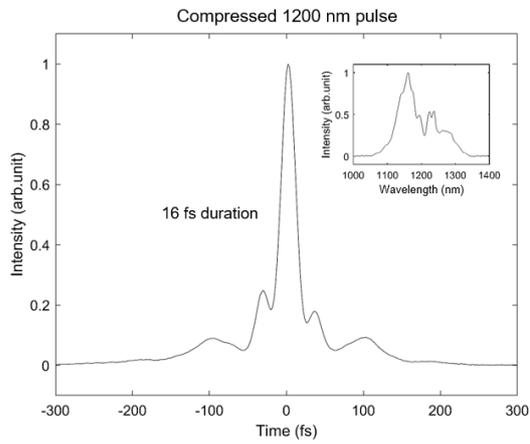
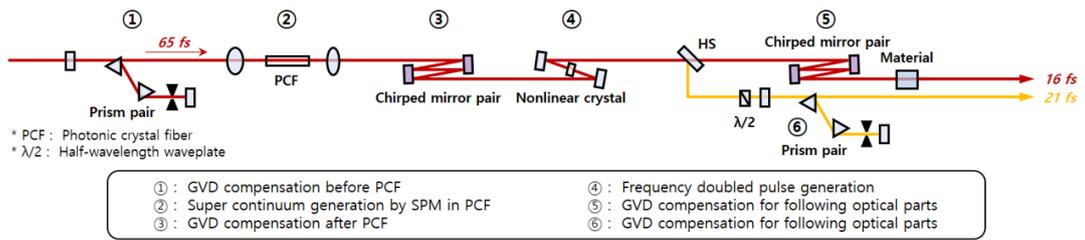
Zoom 8 FRI 15:00~16:00

Generation of sub-20 fs pulse at 1200 nm using pulse compression with a photonic crystal fiber and its application to time-resolved fluorescence

Munnyon Kim, Taiha Joo*

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

For time-resolved spectroscopy with high time resolution, it is necessary to obtain a short pulse with well-defined phase. Here, we performed the pulse compression using a nonlinear effect in the photonic crystal fiber (PCF) and group velocity dispersion (GVD) compensation. We injected a 65 fs duration pulse with 1200 nm center wavelength into the PCF, and obtained spectrally broadened pulse. By performing GVD compensation using chirped mirror pair and material dispersion, we obtained the compressed pulse with 16 fs time duration. The pulse shape is not perfectly Gaussian; there are some minor peaks, impossible to remove by GVD compensation, around the main peak. We performed frequency doubling of the compressed pulse and obtained a 21 fs pulse duration at 600 nm, without the artifacts. Time-resolved fluorescence (TF) based on up-conversion technique was also performed using the compressed pulses. The 600 nm pulses (21 fs) and 1200 nm pulses (16 fs) were used as pump and probe, respectively. The time resolving power of the newly constructed TF setup is 35 fs. The artifacts originated from imperfect 1200 nm probe pulse also appeared on the instrument response function (IRF).



Poster Presentation : **PHYS.P-312**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Integrated technique of pulsed laser irradiation and sonochemical processes for the production of highly surface-active NiPd spheres

Yiseul Yu, Seung Jun Lee, Theerthagiri Jayaraman, Shreyanka Shankar Naik¹, Sang Hun Yeon², Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

¹*Chemistry, Gyeongsang National University, Korea*

²*Gyeongsang National University, Korea*

The development of highly surface-active nano-sized and submicron particles with well-defined features is a promising approach in regulating various physicochemical properties of materials for different applications. A new hybrid technique involving pulsed laser irradiation and sonochemical processes for the production of Pd nanoparticles, NiPd alloys, and ZnO and Ag/graphene oxide (GO) composites was developed herein. An unfocused pulsed laser (neodymium-doped yttrium aluminum garnet [Nd:YAG] laser pulse with a wavelength of 532 nm) was used to irradiate a mixture of colloidal Ni solution obtained by ablation and PdCl₂, resulting in the formation of highly surface-active NiPd under continuous sonication at 40 kHz. The physicochemical properties of the synthesized materials were analyzed by X-ray diffraction (XRD), ultraviolet–visible (UV–vis) spectroscopy, field-emission scanning electron microscopy (FESEM), energy-dispersive X-ray spectroscopy (EDS), high-resolution transmission electron microscopy (HR-TEM), and dynamic light scattering (DLS). To investigate their potential uses, the alloys were employed as electrocatalysts in the hydrogen evolution reaction (HER). Notably, the NiPd synthesized by the integrated process exhibited higher HER activity in a 1 M KOH solution (overpotential of 38 mV at 1 mA/cm²) than the material obtained via pulsed laser irradiation alone (44 mV). The enhanced HER performance of the NiPd alloy was attributed to the synergistic effects of the integrated pulsed laser irradiation and sonochemical processes, affording NiPd particles displaying active surface defects and shape homogeneity. These features resulted in high electronic conductivity and low internal resistance of the material. The proposed hybrid technique could be utilized in the upscaling production of various functional materials with controlled properties.

Poster Presentation : **PHYS.P-313**

Physical Chemistry

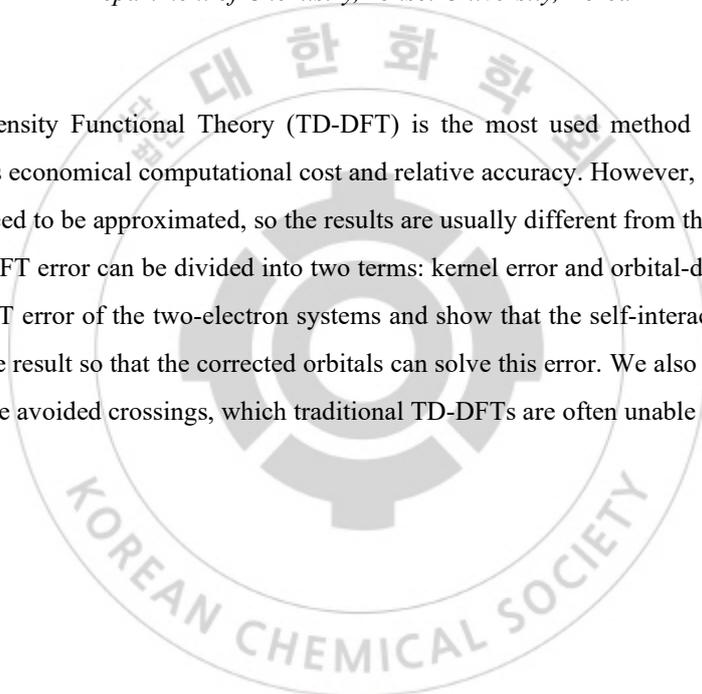
Zoom 8 FRI 15:00~16:00

TD-DFT error decomposition

Hansol Park, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

Time-dependent Density Functional Theory (TD-DFT) is the most used method for excited states of molecules due to its economical computational cost and relative accuracy. However, exchange-correlation (XC) functionals need to be approximated, so the results are usually different from the high-level ab-initio results. Total TD-DFT error can be divided into two terms: kernel error and orbital-driven error. Here, we analyze the TD-DFT error of the two-electron systems and show that the self-interaction error of the XC functional spoils the result so that the corrected orbitals can solve this error. We also discuss the effects of the two errors on the avoided crossings, which traditional TD-DFTs are often unable to predict.



Poster Presentation : **PHYS.P-314**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Pulsed laser assisted synthesis of Pt/C nanocatalysts in various solvents and their electrochemical characterization towards hydrogen evolution reaction.

Yujeong Jeong, Yiseul Yu, Hyecheon Lee, Theerthagiri Jayaraman, Seung Jun Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Robust electrocatalysts toward the resourceful and sustainable generation of hydrogen by splitting of water via electrocatalytic hydrogen evolution reaction (HER) are a prerequisite to realize high-efficiency energy research. Highly electroactive catalysts for hydrogen production with ultralow loading of platinum (Pt) have been under exhaustive exploration to make them cutting-edge and cost-effectively reasonable for water splitting. Herein, we report the one-step synthesis of carbon decorated Pt nanoparticles using pulsed laser ablation (PLA) of Pt target in various solvents such as water, methanol, ethanol, propanol and hexane. The effect of solvent on the size of Pt NPs and carbon layer was investigated systematically. The synthesized Pt/C electrocatalysts was analytically characterized by using various techniques viz., UV-vis, FE-SEM, HR-TEM, and Raman spectroscopy. Voltammetry and Tafel polarization methods have been utilized to assess the performance of various Pt/C catalysts towards hydrogen evolution. Detailed electrochemical investigations revealed that the Pt/C obtained from ethanol solvent exhibits an enhanced HER activity in acidic medium. Therefore, this study revealed a low-cost and single-step production of Pt/C as a promising electrocatalysts for the commercial Pt/C electrocatalysts.

Poster Presentation : **PHYS.P-315**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Pulsed laser-assisted synthesis of metal and nonmetal-codoped ZnO for efficient photocatalytic degradation of Rhodamine B under solar light irradiation.

Sang Hun Yeon, Shreyanka Shankar Naik¹, Seung Jun Lee², Talshyn Begildayeva², Tae Ho Kim², Myong Yong Choi^{2,*}

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Solar light-active silver nanoparticle (Ag NP) and nonmetal nitrogen (N)-codoped zinc oxide (ZnO:N/Ag) nanocomposites were fabricated by a pulsed laser-assisted method. N was considered as a promising candidate for tailoring the bandgap of ZnO due to the similar atomic radius as well as lower ionization energy and electronegativity compared to oxygen, which resulted in the formation of a shallow acceptor level in ZnO. Moreover, Ag NPs could enhance the optical properties of the ZnO materials as a consequence of the surface plasmon resonance (SPR) effect. The synthesized ZnO:N/Ag composite materials were characterized by X-ray diffraction (XRD), micro-Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), field emission scanning electron microscopy (FE-SEM), high-resolution transmission electron microscopy (HR-TEM), energy-dispersive X-ray spectroscopy (EDS), UV-vis diffuse reflectance spectroscopy (UV-DRS), and photoluminescence (PL) analysis. The photocatalytic activity of the ZnO:N/Ag materials was evaluated for the efficient degradation of Rhodamine B (Rh.B) under solar light irradiation. The optimized ZnO:N/Ag-2 nanocomposite exhibited six times higher Rh.B degradation rate than pure ZnO. This was attributed to the enhanced absorption behavior in the solar region as well as the formation of the Schottky junction between ZnO:N and Ag NPs, which resulted in effective charge separation. In addition, the scavenger study revealed that $\cdot\text{O}_2$ radicals facilitated the degradation of Rh.B. The reusability test of the ZnO:N/Ag nanocomposite confirmed high photostability and efficiency of the material in each successive cycle. The present investigation illustrates a rational design of metal and nonmetal-codoped ZnO nanostructures employing a pulsed laser-assisted technique for effective application in photocatalytic remediation of wastewater.

Poster Presentation : **PHYS.P-316**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Cryogenic Ion Spectroscopy of DYYVVR: Structural Assignment by DFT Calculation

Gyeong Ok Song, Jang Han Kwon, Hyuk Kang^{1,*}

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The density functional theory (DFT) is a popular and powerful method for predicting molecular structures with a good balance between computational cost and accuracy. Here we performed a DFT study with harmonic frequency analysis to assign peptide structures. Our group recently reported the cold ion spectroscopy of singly protonated DYYVVR, a tryptic peptide from the active site of Janus kinase 3 (JAK 3), and its point mutants DFYVVR, DYFVVR, DpYYVVR, and DYpYVVR. Comparison of their UV photodissociation spectra shows a tentative evidence that the two tyrosine chromophores lie in distinct solvation environments. IR-UV depletion spectra show that singly protonated DYYVVR has at least two conformers and they have a common hydrogen-bonding pattern with only two different hydrogen-bonding characters. In order to assign its structure, we have performed conformational search at the molecular mechanics level. Then by using a home-made clustering algorithm, we grouped structures to remove duplicated conformations resulted from defects of molecular mechanics and valine residue rotamers. We found 231 groups of structures via the clustering algorithm and 29 candidates were selected from group representatives. We performed geometry optimizations and frequency analyses for these candidates at the ω B97XD/cc-pVDZ level of theory and compared their vibrational frequencies with the IR-UV depletion spectra. Based on these spectra, one conformer is expected to have a hydrogen-bonded carboxylic OH stretch with no free NH stretch in N-terminal, and the other conformer is expected to have free NH stretch in N-terminal with free carboxylic OH stretch. As the system of interest is too large to be searched for all possible conformers, we could find only one structure that had the common hydrogen-bonding pattern. Starting from the found structure, we slightly modified it to have different hydrogen-bonding features mentioned above and performed geometry optimization and vibrational analysis. One structure containing hydrogen-bonded carboxylic OH was successfully optimized and its frequency analysis data could explain the IR-UV spectra.

Poster Presentation : **PHYS.P-317**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

A study on the hydrogen generation reaction over noble metal-free electrocatalyst fabricated by pulse laser assisted technique

Yeryeong Lee, Yewon O, Chae Eun Park, Theerthagiri Jayaraman, Seung Jun Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

The production of sustainable clean energy has become one of the most persistent and significant problems of the current century due to the increasing growth of human population. In order to meet the energy demands, hydrogen is considered to be the best clean fuel for future needs. As a substitute of fossil fuels, hydrogen is readily produced by an electrocatalytic water splitting. The conventional electrocatalysts based on noble metals are scarce and considerably expensive for large-scale hydrogen production, necessitating the search for low-cost earth abundant alternatives. Therefore, we intend to make an effective electrocatalytic materials using pulsed laser ablation as a quick and non toxic techniques without using of any reducing or surfactant. Thus, the fabricated materials is characterized by various analytical techniques such as UV-vis, X-ray diffractometer (XRD), Raman, and scanning electron microscopy (SEM). In addition, the electrocatalytic performance towards the production of hydrogen is evaluated through cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS) analysis.

Poster Presentation : **PHYS.P-318**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Effect of Pulsed Laser Fluence on the Morphology of MoS₂ Nanoparticles

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Molybdenum disulfide (MoS₂), which is a two-dimensional layered material composed of S-Mo-S atomic layers held together by van der Waals interaction, has been recognized as one of the promising candidates for photocatalysts in pollutant decomposition and hydrogen evolution reaction. 2D MoS₂ can be prepared by various methods including mechanical exfoliation, chemical vapor deposition (CVD), liquid-phase exfoliation, wet chemical synthesis, and so on. It has been reported that spherical MoS₂ nanoparticles are produced when MoS₂ target is irradiated by nanosecond laser pulses in liquid phase. The formation of spherical MoS₂ is attributed to the melting of MoS₂ during laser ablation and subsequent solidification of molten liquid droplets. In this study, we investigated the morphology change of MoS₂ nanoparticles dispersed in distilled water under the irradiation of nanosecond laser pulses with varying laser power and fluence. We found that specific intensity of laser is required to melt MoS₂ over a certain size under the same wavelength and irradiation time. By irradiating the nanoparticles with the same amount of total energy but with different fluence and irradiation time, it was found that the peak power, not the total amount of energy, determines the morphology. Despite the distinct shape changes, the initial bulk-phase structure (2H-MoS₂) were almost intact. Irradiation with a relatively low fluence laser could induce the exfoliation of MoS₂ into few-layer nanosheets in a certain type of MoS₂ nanomaterial but not in the other. We explain the difference between two types of MoS₂ as the morphology of the starting materials and the interlayer binding energy. In addition, we will compare the photodegradation efficiency of the laser irradiated MoS₂ with different fluence.

Poster Presentation : **PHYS.P-319**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Cryogenic Ion Spectroscopy of DYYVVR: Structural Assignment by IR Spectroscopy

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Janus kinase 3 (JAK3) is a tyrosine kinase involved in cell signaling, whose activity is regulated by autophosphorylation of its twin tyrosine residues (Y980 and Y981). We have performed cryogenic ion spectroscopy (CIS) of singly protonated DYYVVR, a tryptic peptide of JAK3 (JAK3979-984) that contains the two tyrosine residues, together with its point mutants (Y980F and Y981F) and phosphorylated peptides (pY980, pY981, and pY980pY981). Two broad bands were observed at 35200 cm⁻¹ and 35450 cm⁻¹ in the UV photodissociation (PD) spectrum of cryogenically cooled DYYVVR. When the UV PD spectrum of DYYVVR was compared with those of point mutants, it was found that the UV absorption of Y980 was located at 35450 cm⁻¹ and that of Y981 at 35200 cm⁻¹. Two IR spectral patterns were observed from IR-UV depletion spectra of DYYVVR, and it is concluded that at least two conformers of the cryogenically cooled peptide coexist in the gas phase. By comparing the IR spectra of DYYVVR with those of point mutants, it was found that the IR absorption of phenolic OH stretch vibration in Y981 (981OH) was observed at 3544 cm⁻¹ and that of Y980 (980OH) was at 3570 cm⁻¹, well separated from each other in both conformers. Hydrogen bonded NH stretch in NH₃⁺ (3170 cm⁻¹) and free OH stretch in COOH (3515 cm⁻¹) exist in conformer A, while hydrogen bonded COOH (3250 cm⁻¹) and free NH in NH₃⁺ (3360 cm⁻¹) exist in conformer B. The 981OH in H₂-tagged IR spectrum of DYYVVR was red-shifted by 6 cm⁻¹ from the one in the IR depletion spectra. Since H₂ is mainly tagged at positive charges such as RNH₃⁺ or ROH₂⁺, it is expected that H₂ is mainly attached to R984 of DYYVVR, and the red-shift of 981OH suggests that Y981 and R984 are interacting with each other in both conformers. Three IR spectral patterns in the IR-UV depletion spectra of DpYYVVR imply that DpYYVVR exist as three conformers in the gas phase at cryogenic temperature. In the case of DYpYVVR, only one IR-UV hole-burning spectrum was found and DYpYVVR seems to exist as one conformer under the experimental condition.

Poster Presentation : **PHYS.P-320**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

KS-pies: An Open-Source Program for Kohn-Sham Inversion

Seungsoo Nam, Eunji Sim*

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Kohn-Sham (KS) density functional theory (DFT) is one of the most widely used electronic structure methods. Nevertheless, present KS-DFTs are all approximations due to the unknown nature of exact exchange-correlation functional. Moreover, the non-interacting particle ansatz of KS-DFT prohibits utilizing density information obtained from high-level calculations. In this regard, KS inversion translates exact information into the KS framework, by obtaining KS potential from any input electron density. Despite the usefulness of KS inversion and several decades of developments, software for routinely performing these calculations was scarcely small. In our open-source software KS-pies, we implemented popular KS inversion algorithms also with various pre-and post-processing of inversion calculations. KS-pies provides user-friendly APIs also with documented code to encourage future development.

Poster Presentation : **PHYS.P-321**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

Machine learning based exchange-correlation functional with decomposed error correction

Eunji Sim^{*}, Sechan Lee

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Kohn-Sham Density functional theory (KS-DFT) is developed to calculate the energy of molecules in a practical way. However, due to its approximated manner for the XC functionals, standard DFT results differ from the exact KS-DFT energy which is called a total error. The total error can be divided into two components: density-driven error and functional error. These two different sources of error make it hard to describe the physical properties when the XC functionals are made up by targeting the total error. Those XC functionals will suffer from the mixing effect between density and functional error which can be seen as a collapse for the response function of the energy, but at least, will give a relatively small total error as shown in Ref. 1. This presentation discusses the implications of using machine learning technology to provide flexibility for constructing XC functionals. 1.S. Song, S. Vuckovic, E. Sim,^{*} K. Burke, "Density Sensitivity of Empirical Functionals," J. Phys. Chem. Lett., 12(2), 800–807 (Jan. 7, 2021).

Poster Presentation : **PHYS.P-322**

Physical Chemistry

Zoom 8 FRI 15:00~16:00

A DFT Study for Single and Bilayer Graphene Material

Youngsam Kim, Eunji Sim*

Department of Chemistry, Yonsei University, Korea

For the past few decades, graphene, a 2D semiconductor, has been one of the most popular materials in solid-state chemistry. Because of its unusual band gap character, its physical properties, including electronic structures, have been well studied, both experimentally and computationally. Among many electronic structure calculation methods, density functional theory (DFT) is often the preferred choice because of its practical cost and sufficiently accurate results compared to experimental results. However, due to the approximate manner of the XC functional, semi-local functionals often fail to take into account the main features of the adsorption process, long-range effects such as van der Waals energy. Since these failures are highly system-dependent, it is important to test the functional dependencies of the calculations. Here, we discuss the XC functional dependency by comparing the optimized structure and the electronic structure for graphene-related materials. Local density approximation (LDA), generalized gradient approximation (GGA), and nonlocal XC functionals are used, including a description of the +U functional.

Poster Presentation : **PHYS.P-323**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

Reaction dynamics of phenyl radical in solution

Yejin Park, Seongchul Park, Manho Lim*

Department of Chemistry, Pusan National University, Korea

The reaction dynamics of phenyl radical in CCl_4 was studied by time-resolved vibrational spectroscopy. Nitrosobenzene and Iodobenzene was used as precursors of phenyl radical. Nitrosobenzene exists in two forms in equilibrium of monomeric and dimeric forms in solution, but only monomer is observed in CCl_4 . When Nitrosobenzene is excited at 300 nm the energy of which exceeds C-N bond dissociation energy of Nitrosobenzene, direct dissociation into NO and phenyl radical occurs. Dynamics of subsequent reaction will be easily probed. In the case of iodobenzene excited by a 267 nm photon, predissociation from the initially excited state to the repulsive state occurs due to spin-orbit coupling. Phenyl radical has characteristic vibrational bands in the spectral region of $1440 \sim 1430 \text{ cm}^{-1}$. By observing this spectral region, the reaction dynamics of the nascent phenyl radical with the surrounding solution as well as the dissociating partner will be probed.

Poster Presentation : **PHYS.P-324**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

CuO and Ni nanoparticles as multifunctional electrocatalysts for energy conversion and storage

Talshyn Begildayeva, Seung Jun Lee, Hyeyeon Lee, Myong Yong Choi*

Department of Chemistry, Gyeongsang National University, Korea

Laser ablation of Cu and Ni metal plates alternately in methanol solution allows production of spherical and rod-like CuO NPs (Ni-CuO and CuO-Ni nanocomposites, respectively). In this work the effect of ablation order of Cu and Ni plates can be seen clearly. When Cu plate is ablated first, the growth of rod-like CuO NPs can be detected. Secondary ablation of Ni NPs does not affect on the final structure of CuO-Ni nanocomposite. However, presence of Ni NPs from first PLAL in methanol inhibits the growth of CuO rods, and keeps it as well-dispersed spheres with diameter of ~30-50 nm. Further, CuO-Ni and Ni-CuO nanocomposites were characterized by UV-visible, XRD, Raman, SEM and TEM analyses. Next, these materials synthesized by PLAL were applied for electrochemical oxidation of methanol. Both materials perform direct oxidation of methanol, what makes them advantageous over noble metal NPs. Composite with spherical CuO NPs exhibited 5 times higher current density compare to that of sample, where CuO NPs appear as rods, and comparable with that of materials synthesized through the conventional methods. This superior performance caused by the more number of available active sites in the Ni-CuO nanocomposite, originating from the size difference of rod-like and spherical CuO NPs. As one of the promising application of these materials, Ni-CuO nanocomposite were tested in hydrogen evolution (HER) and oxygen evolution reactions (OER) in alkaline media. It is the first report, where material prepared by laser ablation was applied as bifunctional electrode for HER and OER. This material can be further studied for water splitting applications in the next works.

Poster Presentation : **PHYS.P-325**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

Laser Assisted Synthesis of ZnS/Au/MWCNT nanostructure for an efficient electrochemical sensing of 4-nitrophenol.

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Myong Yong Choi^{1,*}**

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¹*Department of Chemistry, Gyeongsang National University, Korea*

²*Gyeongsang National University, Korea*

Herein, we have successfully synthesized ZnS /Au/MWCNT nanostructure by performing pulsed laser assisted and wet-chemical technique. The diverse nature of materials such as ZnS , Au and MWCNT with quantified ratio of nanomaterials could be exploited for an efficient electrochemical sensor for the detection of 4-nitrophenol (4-NP). The as prepared material and their compositions were well characterized using X-ray diffraction, field emission scanning electron microscopy (FE-SEM), high resolution transmission electron microscopy (HR-TEM), and UV-visible absorbance spectroscopy analysis. The optimized ZnS/Au10wt%/MWCNT3wt% nanostructure modified on GCE electrode showed an enhanced electrocatalytic response towards 4-NP detection. The optimized ZnS/Au10wt%/MWCNT3wt% nanocomposite exhibit the limit of detection (LOD) of 0.115 uM at pH-5 using Linear Sweep Voltammetric method. Moreover, the effects of scan rate and pH range were well examined to find out the optimized conditions at which there were a higher sensitivity and low detection limit. An appreciable precision was found towards the stability of the assay in the determination.

Poster Presentation : **PHYS.P-326**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

Design, synthesis fluorometric chemosensor of phenylalanine derivative for selective Cu(II) detection

Hyang-Im Ryou, Ki Hwan Lee*

Department of Chemistry, Kongju National University, Korea

A novel fluorescent chemosensor DPB was designed, synthesized, and characterized based on phenylalanine bearing 2-amino-6-methylbenzothiazole at the side chain functionalized with electron donor group and dansyl chloride as a fluorophore. Chemosensor DPB was showed selectivity for Cu(II) ions among 17 metal ions in aqueous solutions. The static fluorescence quenching led to form non-fluorescent complexation of chemosensor DPB and Cu(II) at 1:1 ligand-metal binding stoichiometry. The binding interaction, nature of fluorescence quenching, and binding stoichiometry are discussed in detail by Job's method, Stern-Volmer plot, and absorption, fluorescence, and lifetime measurements.

Poster Presentation : **PHYS.P-327**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

Energetics of the Surfactant Micelle Deformation on the Surface of Ceramide and Phospholipid Membranes via Molecular Dynamics Simulations

Yeonho Song, Hyonseok Hwang*

Department of Chemistry, Kangwon National University, Korea

Free energy variations and deformations of surfactant (sodium lauryl ether sulfate, SLES) micelles near the surface of ceramide24:0 (Cer240) and the phospholipid (1,2-dimyristoyl-*sn*-glycero-3-phosphorylcholine, DMPC) bilayers are investigated using molecular dynamics (MD) simulations and 2D potential of mean force (2D-PMF) calculations. In the previous constant-force steered molecular dynamics (cf-sMD) study, a SLES micelle exhibited different shapes on the Cer240 and the DMPC bilayers: an upper hemispherical shape in the Cer240 bilayer and a spherical shape with more hydrophilic head groups populated in the lower part of the sphere in the DMPC bilayer.¹ To look into the distinct behavior of the SLES micelle near the surface of the Cer240 and DMPC bilayers more closely, we constructed 2D-PMF profiles as a function of distance between the center of mass (CoM) of the micelle and the center of the bilayer and micelle deformation parameter. Indeed, the 2D-PMF profiles reveal why a SLES micelle has different shapes on the Cer240 and the DMPC bilayer

1. Y. Song, J. H. Lee, I. Jung, B. Seo, and H. Hwang, "Molecular Dynamics Simulations of Micelle Properties and Behaviors of Sodium Lauryl Ether Sulfate Penetrating Ceramide and Phospholipid bilayers", *J. Phys. Chem. B* **124**, 5951 (2020).

Poster Presentation : **PHYS.P-328**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

A New Method Based on Machine Learning Algorithm to Calculate Reaction Field Energy in Model Ion Channels

Inhyeok Choi, Hyonseok Hwang*

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The reaction field energy (RFE), which was previously obtained through the Poisson-Boltzmann equation (PBE) and basis-set expansion (BSE) methods in the Kinetic Lattice Grand Canonical Monte Carlo simulation combined with mean field theory (KLGCMC/MF simulation) is calculated using a linear regression model based on an artificial neural network (ANN) algorithm.¹ The criteria for evaluating the trained ANN were largely determined in two methods. The first method is to calculate the R^2 score between the predicted energy and the exact energy in the linear regression model. In the second method, the accuracy was defined as the number of the predicted RFEs within 10% of the exact RFE values and the accuracy was compared between the ANN and BSE methods. The R^2 score obtained from the ANN algorithm was 0.988, which is higher than 0.970 from the BSE method. In addition, the accuracy of ANN, 29%, is also higher than that of the BSE method where the accuracy was 22%. In particular, the ANN algorithm predicted the RFE with higher accuracy than the BSE method when there is no ion inside a model ion channel even though the training data set for a system where at least one ion exists inside the ion channel was used. In this respect, the proposed ANN algorithm is considered suitable for the calculation of RFEs in an ion channel system.

1. H. Hwang, G. C. Schatz, and M. A. Ratner, Kinetic Lattice Grand Canonical Monte Carlo Simulation for Ion Current Calculations in A Model Ion Channel System, *J. Chem. Phys.* **127**, 024760 (2007).

Poster Presentation : **PHYS.P-329**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

The charged state of glutamic acid has a significant impact on its transport through cyclic peptide nanotubes

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In this study, molecular dynamics (MD) simulations were used to investigate the transport mechanism of glutamic acid through a cyclic peptide nanotube (CPN), 8x cyclo[-(Trp-D-Leu)₄-Gln-D-Leu-] in DMPC double layers. In particular, the effect of the three different charged states of glutamic acid such as anionic, zwitterionic, and cationic forms on the transport through CPNs were thoroughly examined by calculating the potential of mean force (PMF) profiles and position-dependent diffusion coefficients of glutamate ions. In the PMF calculations, energy barriers of nearly 20 kcal/mol are observed for anionic form of glutamic acid while energy wells of -10 kcal/mol are shown for cationic form, indicating that CPNs are cation-selective due to carbonyl oxygens inside the CPNs. The PMF decomposition profiles illustrate that the anionic form of glutamic acid has favorite interactions with water molecules, but the interactions with water molecules inside the channel fail to compensate for repulsive interactions of anionic glutamate with the CPN and DMPC bilayer. On the other hand, the cationic form of glutamic acid possesses attractive interactions with the CPN and DMPC bilayers that overcome the repulsive interactions with water molecules. The zwitterionic form shows moderate interactions with CPN, DMPC, and water molecules. While the PMF profiles differ among the three charged forms of glutamic acid, distinct difference in the position-dependent diffusion coefficients of glutamate ions inside the CPN are not observed. Finally, hydrogen bonding calculations demonstrate that the negative form of glutamic acid loses the largest number of hydrogen bonds inside the CPN among the three charged states while the number of hydrogen bonds in the positive form slightly decreases through the CPN.

Poster Presentation : **PHYS.P-330**

Physical Chemistry

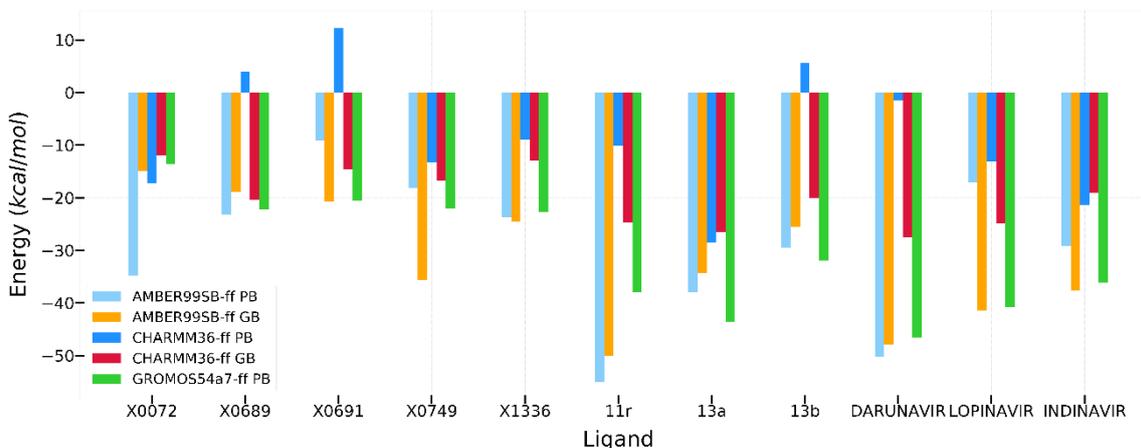
Zoom 8 FRI 16:00~17:00

Identifying the hot spots of the SARS-CoV-2 main protease by using a series of different force field

Jinyoung Byun

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Recently the coronavirus, SARS-CoV-2 has caused numerous infections and death. However, as there is no enough experimental material, it prevents identifying the therapeutic remedy to handle the COVID-19. So it is inevitable to discover a new effective drug to treat the COVID-19. Here we show the MM-PB/GBSA analysis results in order to inspect the correlation between a series of force fields. We selected SARS-CoV-2 main protease(Mpro) as a target receptor and ligands with a series of force field, GROMOS54a7 force field, AMBER99SB force field, and CHARMM36 force field to investigate their dynamics with interesting ligands on each force field, followed by analyzing which Mpro's residues are attributed to the binding energies by using 'MM-PB/GBSA' analysis. MM-PB/GBSA analysis allows us to fast identify which residues are hotspots which have binding energy -1.0 kcal/mol in the drug discovery process. Through MM-PB/GBSA analysis, we inspected whether the overall binding energy's trend between the Mpro-ligands complex exists or not and also identified which Mpro residues more contributed to the binding energy via binding energy decomposition per residue.



Poster Presentation : **PHYS.P-331**

Physical Chemistry

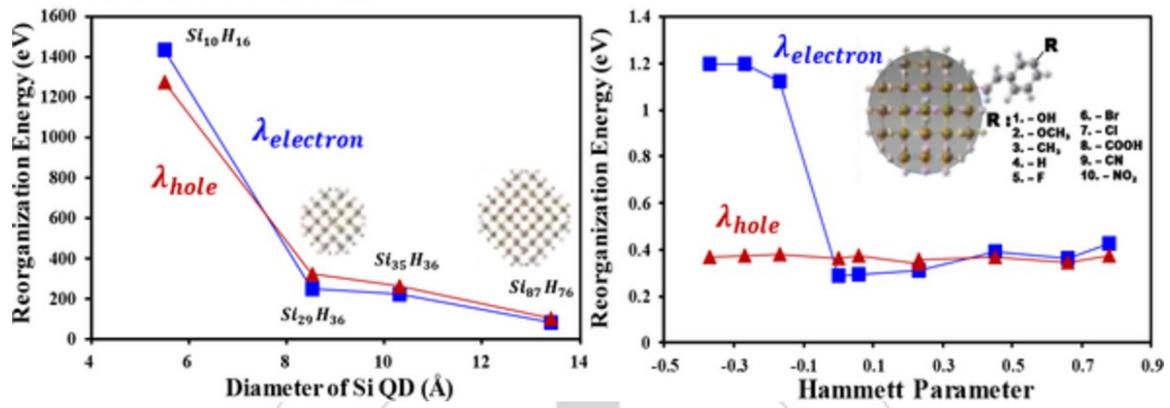
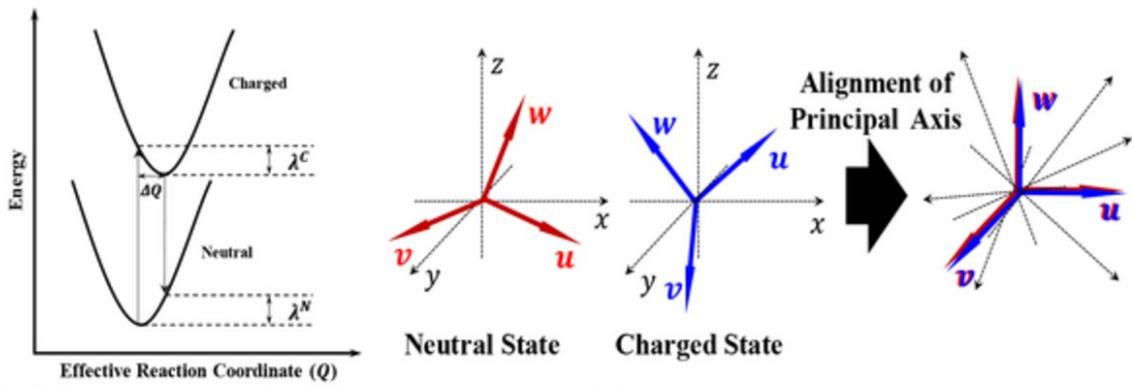
Zoom 8 FRI 16:00~17:00

Development of a MATLAB Algorithm for Calculating Reorganization Energy Utilizing Rectilinear Normal Mode Displacements: The Effect of Substituents on Reorganization Energies of Styryl-Capped Silicon Quantum Dots

Young-Hwa Choi, Hyeok Yun, Hyun-Dam Jeong*

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We developed a MATLAB algorithm to calculate reorganization energy utilizing rectilinear normal mode displacements. Normal mode-projected rectilinear displacements and the corresponding angular frequencies, required for evaluating charge transfer reorganization energy within the harmonic oscillator approximation, were obtained from Cartesian coordinates and Cartesian force constant matrices determined with respect to the principal axes. To verify the algorithm developed with MATLAB, we compared the computed charge transfer reorganization energies to those evaluated by the DUSHIN program, and there was no substantial difference, indicating that our algorithm guarantees the numerical accuracy of the calculations. This algorithm was applied to design silicon quantum dots (Si QDs) with low reorganization energies for charge transfer.



Poster Presentation : **PHYS.P-332**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

Quantum Chemical Calculation of Electronic Coupling for Studying Non-adiabatic Electron Transfer in Molecule-Bridged Silicon Quantum Dot Dimer System

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Understanding the electronic coupling in molecule-bridged semiconductor quantum dot (QD) dimer system is of great importance not only from a fundamental perspective on non-adiabatic electron transfer, but also from the development of semiconductor QD-based optoelectronic devices. In this work, we present a quantum chemical theoretical approach and computational details for the electronic coupling between QDs in molecule-bridged QD dimer system using a segmented AO-based Fock matrix for donor, bridge, and acceptor. A computing platform implementing a theoretical approach for evaluating the electronic coupling was developed with MATLAB R2018b. The input for the computing platform was obtained from quantum mechanical calculations performed with the Gaussian 16 program package. The geometric optimization and Fock matrix construction of molecule bridged Si QD dimer systems was carried out at the DFT level using the 6-31G(d,p) basis set. Becke's three parameter gradient-corrected exchange potential and the Lee-Yang Parr gradient-corrected correlation potential (B3LYP) were used for all the calculations. The MATLAB computing platform for calculating the electronic coupling between silicon quantum dots (Si QDs) in molecule-bridged QD dimer system was applied to understand the modulation of electronic coupling depending on the diameter of Si QDs and the structure of the bridged molecules. The evaluation of electronic coupling in molecule-bridged QD dimer system can be used to estimate the electrochemical properties of molecule-bridged Si QD cluster, our newly proposed concept of anode material.

Poster Presentation : **PHYS.P-333**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

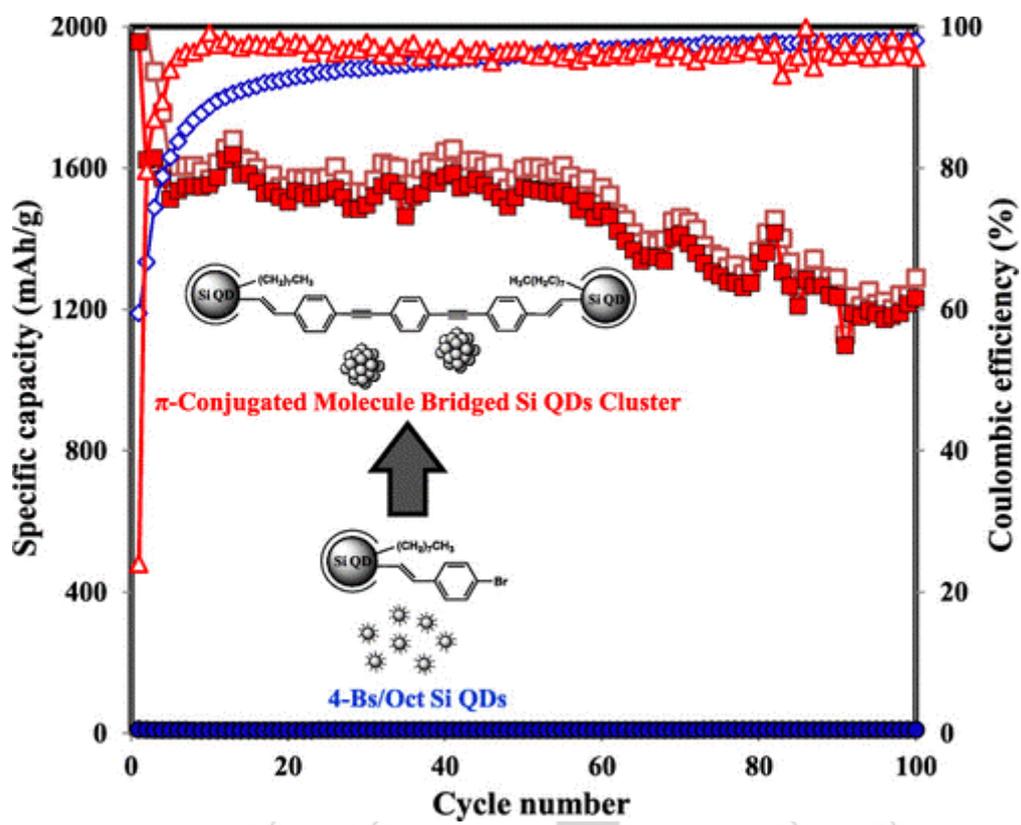
Synthesis and Electrochemical Performance of π -Conjugated Molecule Bridged Silicon Quantum Dot Cluster as Anode Material for Lithium-Ion Batteries

Young-Hwa Choi, Hyeonbeom Park¹, Hyun-Dam Jeong^{*}

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¹*Chemistry, Chonnam National University, Korea*

π -Conjugated molecule bridged silicon quantum dots (Si QDs) cluster was prepared by Sonogashira C-C cross-coupling reaction between 4-bromostyryl and octyl co-capped Si QDs (4-Bs/Oct Si QDs) and 1,4-diethynylbenzene. The surface chemical structure, morphology, and chemical composition of the Si QDs cluster were confirmed by Fourier-transform infrared spectroscopy, field-emission transmission electron microscopy, and energy-dispersive X-ray spectroscopy. Lithium ion batteries were fabricated using the 4-Bs/Oct Si QDs and the Si QDs cluster as anode materials to investigate the effect of QDs clustering on the electrochemical performance. Compared with the 4-Bs/Oct Si QDs electrode, the Si QDs cluster exhibits improved electrochemical performance, such as the high initial discharge capacity of ~ 1957 mAh/g and good cycling stability with ~ 63 % capacity retention following 100 cycles at a current rate of 200 mA/g when tested at the voltage window of 0.01~2.5 V. The improved electrochemical performance of the Si QDs cluster is attributed to the π -conjugated molecules between the Si QDs and on the surface of Si QDs cluster, which serve as a buffer layers to alleviate the mechanical stresses arising from the alloying reaction of Si with lithium, and maintain the electrical conduits in the anode system.



Poster Presentation : **PHYS.P-334**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

The dynamics of bimolecular proton transfer in aqueous solution using Time-resolved Vibrational spectroscopy

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The neutralization of an acid by a base is one of the fundamental reactions in solutions. We observed aqueous bimolecular proton transfer, using a photoacid, 8-hydroxy-1,3,6-trisulfonate-pyrene (Pyranine, PyOH), which reacts with azide (N_3^-) as a strong acid when electronically excited. The most significant IR spectra changes of PyOD between electronic ground-state and excited-state occur in the spectral region of 1400-1650 cm^{-1} . Azide has a strong band at 2042 cm^{-1} and its conjugated acid (DN_3) at 2133 cm^{-1} . Time-resolved vibrational spectra were measured in these spectral regions after excitation of PyOH in the presence of N_3^- in D_2O solution with a 400-nm pulse. In the presence of low base concentration (< 150 mM of N_3^-), the dominant reaction path was found to be the bimolecular reaction between the base molecule and deuteron (D^+) which was dissociated from the excited state PyOD, rather than direct reaction from acid-base complexes that was observed in high base concentration. The bimolecular reaction involved in acid-base reaction observed via this research will be presented.

Poster Presentation : **PHYS.P-335**

Physical Chemistry

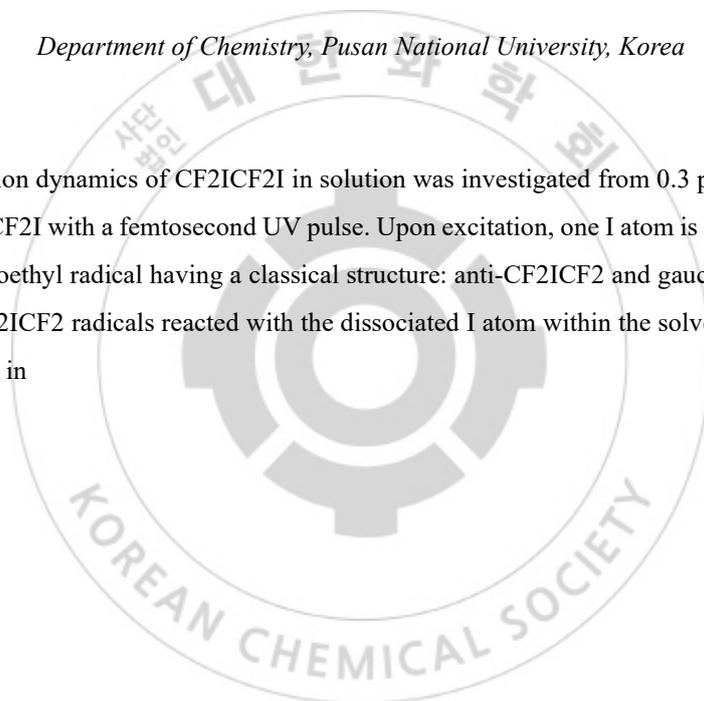
Zoom 8 FRI 16:00~17:00

Conformer-Specific Photodissociation Dynamics of CF₂ICF₂I in Solution Probed by Time-Resolved Infrared Spectroscopy

Seongchul Park, JuHyang Shin, Hojeong Yoon, Manho Lim*

Department of Chemistry, Pusan National University, Korea

The photodissociation dynamics of CF₂ICF₂I in solution was investigated from 0.3 ps to 100 μs, after the excitation of CF₂ICF₂I with a femtosecond UV pulse. Upon excitation, one I atom is eliminated within 0.3 ps, producing a haloethyl radical having a classical structure: anti-CF₂ICF₂ and gauche-CF₂ICF₂. All the nascent gauche-CF₂ICF₂ radicals reacted with the dissociated I atom within the solvent cage to produce a complex, I₂·C₂F₄, in



Poster Presentation : **PHYS.P-336**

Physical Chemistry

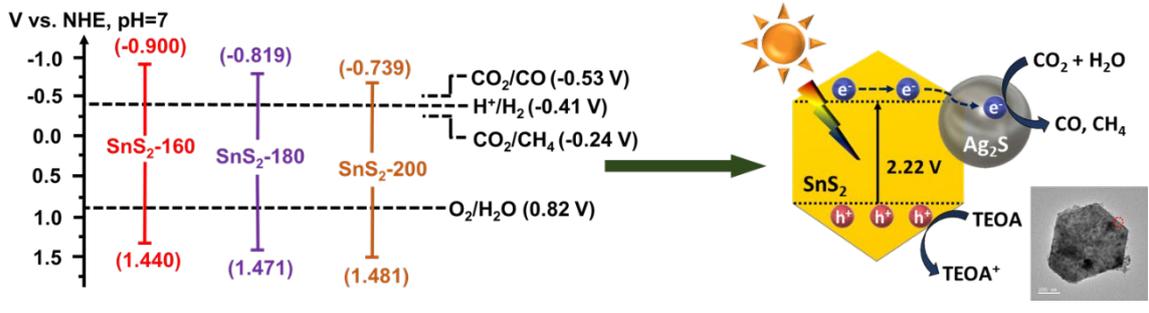
Zoom 8 FRI 16:00~17:00

Silver sulfide quantum dots supported two-dimensional tin disulfide for photocatalytic carbon dioxide reduction under solar light

Putta Rangappa, Praveen Kumar Dharani, Tae Kyu Kim*

Department of Chemistry, Yonsei University, Korea

In this study, we fabricated highly efficient plate-like SnS₂ nanostructures via the facile hydrothermal (HT) method and unravel the effect of temperature on photo-physical properties. The SnS₂ synthesized at 200 °C disclosed the presence of a highly distributed plate-like structure and which showed an enhanced photo-physical property for catalytic reactions. Further, the shorter diffusion path length with maximum exposed facets of the highly dispersed plate-like structures are responsible for boosted photocatalytic CO₂ reduction reactions. Next, the optimized SnS₂ was decorated with Silver sulfide (Ag₂S) quantum dots by a simple cation exchange process in the water at room temperature. The obtained composites were employed for the assessment of photocatalytic CO₂ conversion in presence of water with the assistance of TEOA as a hole scavenger. The optimized SnS₂/Ag₂S-50 showed highly efficient CO₂ reduction and the cumulative yields of CO and CH₄ has reached 744.96 μmol g⁻¹ and 24.64 μmol g⁻¹ respectively in 16 h of time course and it is ~7 folds higher than the pristine SnS₂-200. Overall, the enhanced activity of SnS₂/Ag₂S-50 was expected from the effective charge transfer of photogenerated charge carriers with layered SnS₂ and the decorated Ag₂S quantum dots showed improved charge separation efficiency, enhanced light-harvesting capacity from visible to IR region and feasible band potentials. The proposed SnS₂/Ag₂S nanohybrid serve as a promising low-cost, stable, and highly efficient catalyst for long-term practical applications of CO₂ reduction reactions under solar light.



Poster Presentation : **PHYS.P-337**

Physical Chemistry

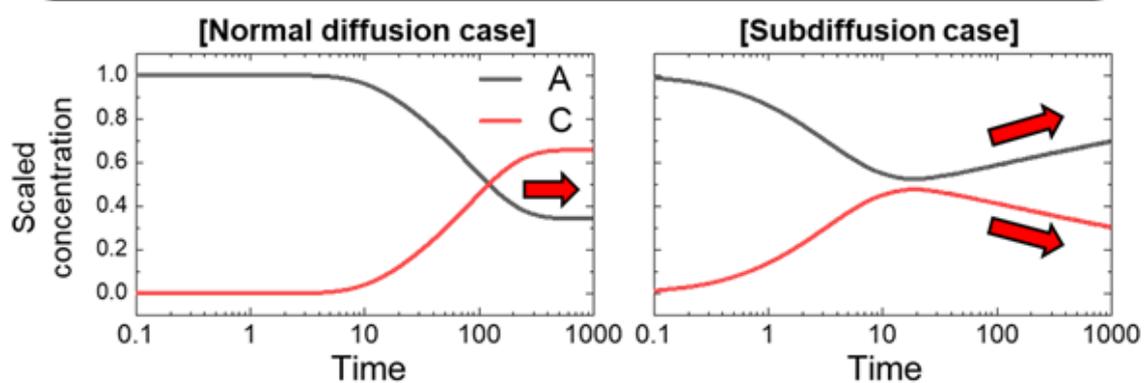
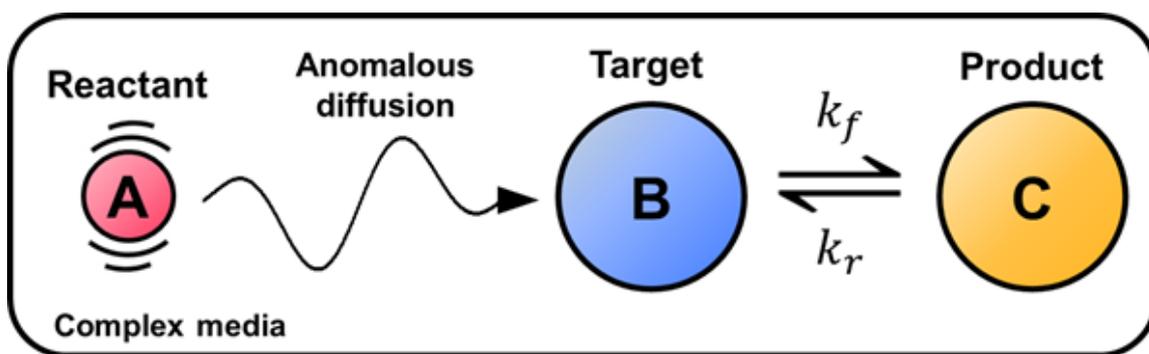
Zoom 8 FRI 16:00~17:00

Subdiffusion-influenced reversible reaction

Min Ho Lee, Ji-Hyun Kim^{*}, Jaeyoung Sung^{*}

Department of Chemistry, Chung-Ang University, Korea

Chemical reactions constantly take place in an organism to maintain its vital functions. In the case of enzymatic reactions, cell signaling, and self-assembly based on chemical reactions, it has been found that the diffusion of molecules has a significant effect on chemical reactions. While there has been extensive work on the role of Fickian diffusion in relation with the diffusion-influenced reversible reaction, there is no theoretical or quantitative understanding of how anomalous diffusion of reactants or products influences reversible reaction, despite many reports that have found that the diffusion of molecules in highly crowded media inside living cells is not Fickian but anomalous. In this work, we investigate diffusion-influenced reaction in the case of subdiffusion as well as Fickian diffusion using a continuous time random walk model in finite space. For the reversible reaction, $A + B \rightleftharpoons C$, we confirm the validity of our theoretical results against accurate computer simulation. For Fickian diffusion, the number of reactants and products reached chemical equilibrium, but for subdiffusion case, our results do not indicate chemical equilibrium and all the products were reduced to reactants in the long-time limit, even if there is a strong attractive potential between reactant species, A and B. We reveal that this apparently paradoxical result is related to transient trapping events of reactants occurring in the case of subdiffusion: rare but deep trapping events cause dwell times on the order of the observation time.



Poster Presentation : **PHYS.P-338**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

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-339**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

BiVO₄ Photoanode Modified by Silver Nanoparticles and Co-Pi For Efficient Photoelectrochemical Water Oxidation

**Kethireddy Arun Joshi Reddy, Madhusudana Gopannagari¹, Praveen Kumar Dharani¹,
Tae Kyu Kim^{1,*}**

Chemistry, Yonsei University, Korea

¹*Department of Chemistry, Yonsei University, Korea*

Photoelectrochemical (PEC) water splitting is a promising and environmentally friendly route for the conversion of solar energy into useful fuels. Sufficient visible light harvesting as well as separation and transport of photogenerated charges play a pivotal role on the photoelectrochemical performance of photoelectrodes. Bismuth vanadate (BiVO₄) has shown great potential for PEC catalysis, but it needs to be further modified because of its inadequate light harvesting, charge separation and transfer efficiencies have harshly limited the photoelectrochemical water oxidation performance. Herein, we modified BiVO₄ photoanode by plasmonic Silver (Ag) nanoparticles and with cobalt phosphate (Co-Pi) to accomplish effective water splitting. In this Co-Pi/Ag-BiVO₄ (CAB) photoanode, the Ag nanoparticles acts as photosensitizers broaden the absorption spectrum and promote charge separation due to its enchanting surface plasmon resonance effect, moreover Co-Pi acts as hole transfer layer which stimulate charge separation and transfer and enhance the stability of photoanode. As a result, the CAB photoanode generate enhanced photocurrent at 1.23 V (vs RHE) under 1.5G illumination in 0.5M Na₂SO₄ electrolyte solution, which is virtually 5 times higher than that of bare BiVO₄. The surface modification approach developed in this work remarkable promotes the photocurrent density of BiVO₄ by facilitating carrier transfer in addition to a charge separation efficiency enhancement.

Poster Presentation : **PHYS.P-340**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

Detection of Amyloid beta-42 on silver Nanoshells Using Surface enhanced Raman spectroscopy

Eungyeong Park, Eun Hae Heo¹, Hyejin Chang^{1,*}

Department of Chemistry, Kangwon National University, Korea

¹Division of science education, Kangwon National University, Korea

The deposition of amyloid beta 42 ($A\beta_{42}$) on the brain has been considered as one of the causes of Alzheimer's disease. Therefore, development of an early diagnosis method with high sensitivity and reliability for the detection of $A\beta_{42}$ is necessary. In this study, we have developed Ag nanoshell-p-aminothiophenol (ATP)- Cu^{2+} system as an $A\beta_{42}$ sensor. When the $A\beta_{42}$ combined with Cu^{2+} due to the strong affinity, then surface-enhanced Raman spectrum of p-ATP was showed the spectral change due to the orientation shift. Details of the results will be discussed in the presentation.

Poster Presentation : **PHYS.P-341**

Physical Chemistry

Zoom 8 FRI 16:00~17:00

Photoinduced energy transfer in polymers bearing π -extended donor and acceptor monomers: The role of linkers

Youngseo Kim, Nayeon Kwon, Dong Hoon Choi*, Sunnam Park*

Department of Chemistry, Korea University, Korea

Photoinduced energy transfer is an important process in solar cells and depends on the morphology of the photoactive layers that is significantly influenced by the molecular structures. In this work, we studied the photoinduced energy transfer dynamics in two polymers, $(D-\sigma-A)_n$ and $(D-\pi-A)_n$ that have different linkers between π -extended donor (D) and acceptor (A) units. $(D-\sigma-A)_n$ polymers have non-conjugated alkyl linkers while $(D-\pi-A)_n$ polymers have π -conjugated linkers. The optical and photophysical properties were studied by UV-visible absorption, emission, and time-resolved fluorescence spectroscopy along with DFT calculations. Both polymers undergo photoinduced energy transfer from donor to acceptor units in solutions and films. In solutions, energy transfer was found to occur more efficiently in $(D-\sigma-A)_n$ than in $(D-\pi-A)_n$. This is because $(D-\sigma-A)_n$ can exist in the folded structure in solutions due to the flexible alkyl linkers and the intramolecular energy transfer occurs more favorably in the folded structure of $(D-\sigma-A)_n$. In films, fluorescence was found to be significantly quenched in both polymers because they underwent both intramolecular and intermolecular energy transfers. The energy transfer rates in solutions and films were determined using a simple kinetic model. Our experimental results show the structural flexibility can affect the photophysical property of D-A type polymers, and the linkers between donor and acceptor units need to be properly selected to design the D-A polymers for their intended use.

Poster Presentation : **PHYS.P-342**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Transport dynamics of synaptic vesicles and its effect on exocytosis in stimulated neuron

Gyunam Park, Ji-Hyun Kim*, Jaeyoung Sung

Department of Chemistry, Chung-Ang University, Korea

Synaptic vesicle motion within presynaptic terminals is an essential process underlying neuronal communication. However, complex vesicle motion and its effects on synaptic transmission are poorly understood. Here, we investigate the motion of individual synaptic vesicles by using three-dimensional tracking. We find the fusion time of synaptic vesicles does not simply increase with their initial distance from the fusion site, despite similar instantaneous speed for all vesicles. We discover the straightness of synaptic vesicle motion to be a crucial factor governing the fusion time and this straightness to be proportional to the mean force on synaptic vesicles induced by neuronal stimulation. We discover general transport equation governing synaptic vesicle motion. We extract several important quantities which can understand transport dynamics of synaptic vesicle moving in strongly heterogeneous environment of presynaptic bouton.

Poster Presentation : **PHYS.P-343**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

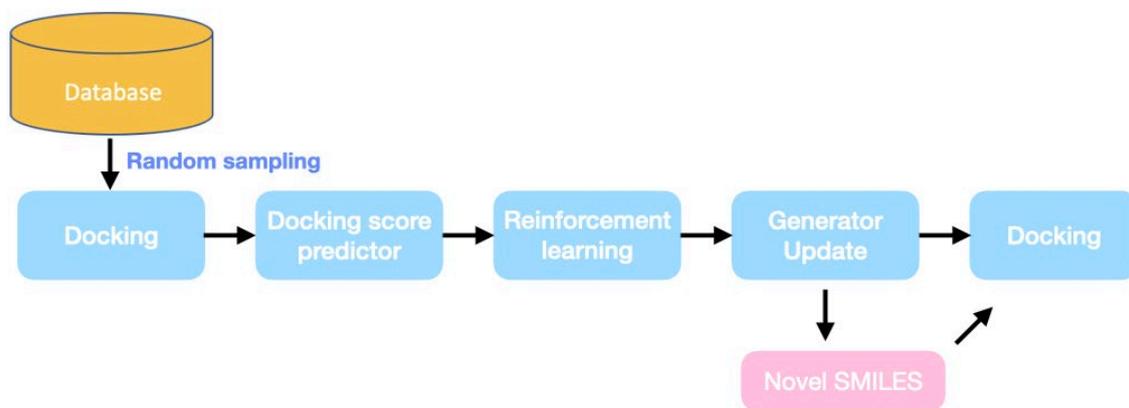
Fast generation of drug-like molecules using machine-learning-based docking score and molecular optimization

Jieun Choi, Juyong Lee^{1,*}

Chemistry, Kangwon National University, Korea

¹*Department of Chemistry, Kangwon National University, Korea*

The goal of drug design is to find novel molecules that have the desired properties, and have benefited greatly from the development of deep learning. In this study, we propose a new molecular design workflow by combining efficient molecular property optimization approaches and molecular docking, which provides heuristics estimation for biological experiments. However, performing docking simulations for all designed molecules explicitly will require significant amount of computational resources. To solve this problem, we utilized a machine-learning-based model that predicts the docking score. By using this workflow, combining molecular docking and molecular optimization approaches, we were able to quickly design molecules with high docking scores for a target protein and molecules with desirable physicochemical properties, a similarity to a reference molecule and a drug-like score, QED. We also show that combinatorial optimization of molecular properties may outperform existing reinforcement-based approaches.



Poster Presentation : **PHYS.P-344**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Machine-learning assisted design of novel fluorescent molecules

Bomin Kim, Juyong Lee^{1,*}

department of chemistry, Kangwon National University, Korea

¹*Department of Chemistry, Kangwon National University, Korea*

In this study, we used and compared multiple machine learning approaches to find novel fluorescent molecules with desired properties. We compared several generative models to generate diverse and distinct novel molecules with desired properties such as high oscillator strength and similarity to a reference scaffold. Three molecular generative algorithms were benchmarked: two reinforcement-learning-based algorithms, ReLeaSE and Molecule Deep Q-Networks (MolDQN), and one combinatorial optimization-based algorithm, MolFinder. By using these algorithms, novel molecules were designed so that a new molecule is similar to a scaffold, has its excitation energy close to a preset value, and high oscillator strength as much as possible. In addition, to design actually synthesizable molecules, the synthetic accessibility score (SAS) is also considered. After molecular design, we performed quantum calculations to validate the accuracy of our design approaches. Among the tested methods, MolFinder showed the best performance. We believe that our results will open new possibilities for ML-assisted molecular design.

Poster Presentation : **PHYS.P-345**

Physical Chemistry

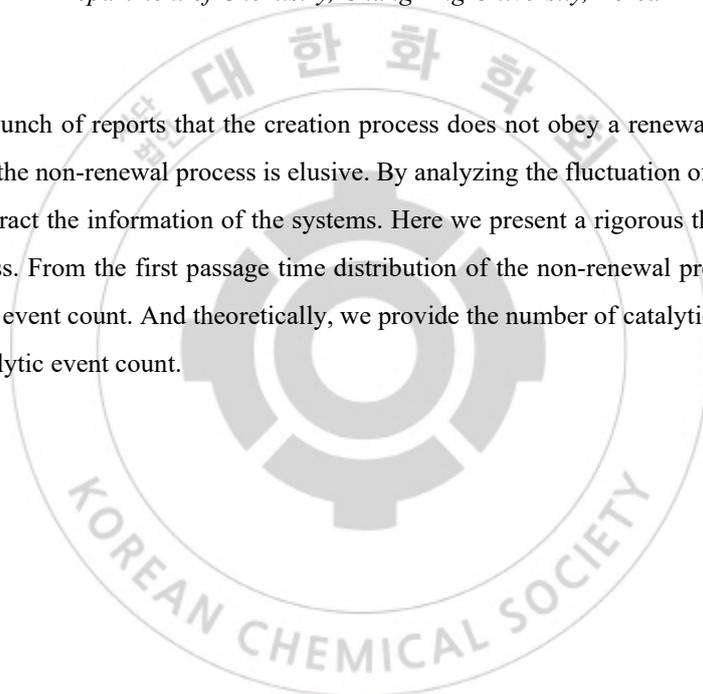
Zoom 9 FRI 15:00~16:00

Stochastic Kinetics of Multi Independent Non-renewal Systems

Heemo Yang, Ji-Hyun Kim^{*}, Jaeyoung Sung^{*}

Department of Chemistry, Chung-Ang University, Korea

While there are a bunch of reports that the creation process does not obey a renewal process, theoretical analysis to explain the non-renewal process is elusive. By analyzing the fluctuation of the creation number of products, we extract the information of the systems. Here we present a rigorous theory of the arbitrary non-renewal process. From the first passage time distribution of the non-renewal process, we investigate the moments of the event count. And theoretically, we provide the number of catalytic sites in terms of the moment of the catalytic event count.



Poster Presentation : **PHYS.P-346**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

The chemical fluctuation theorem governing expression, protein maturation and annihilation

Jin Hyung Kim, Ji-Hyun Kim^{*}, Jaeyoung Sung^{*}

Department of Chemistry, Chung-Ang University, Korea

Fluorescence protein is a powerful probe of gene expression dynamics in living cells. It is known that these protein emit fluorescence after slow maturation processes; however, it is not known how this maturation process affects the protein level which can be probed by fluorescent proteins. Here, we address this issue by presenting a new type of the chemical fluctuation theorem (CFT) that exactly holds for proteins with general gene expression and maturation dynamics. Using the CFT, we present the first, accurate relationship between the gene expression and maturation dynamics to experimental observables including the mean and variance of matured protein level in living cells. We also investigate how dynamic, cell-to-cell fluctuation of the gene expression dynamics and non-exponential lifetime distributions of protein affect these experimental observables. This work enables accurate, quantitative understanding of gene expression and protein maturation dynamics in living cells.

Poster Presentation : **PHYS.P-347**

Physical Chemistry

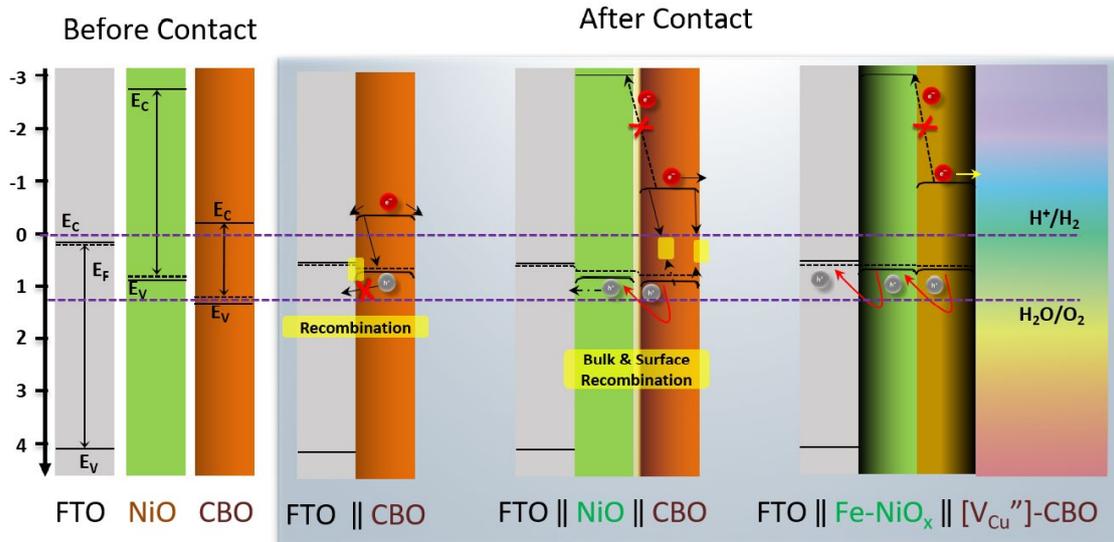
Zoom 9 FRI 15:00~16:00

Augmented CuBi₂O₄ Photocathode: Prominence of Cu-Vacancies and Hole Selective Layer

Madhusudana Gopannagari, Tae Kyu Kim^{*}

Department of Chemistry, Yonsei University, Korea

Electrochemical synthesis methods were developed to produce CuBi₂O₄ (CBO), a promising p-type oxide for use in solar water splitting, due to its exceptional structural, optical band gap alignment, and more positive onset potential. However, despite these favorable attributes, CBO photocathodes have shown limitations in charge carrier transport within CBO and across the interface with n-type fluorine-doped tin oxide (FTO). To overcome both limitations, a very thin doped-NiO_x layer inserted between the FTO and the CBO photocathode, since the importance of NiO is recently described as one of the capable hole transfer layers (HTL) for its hole-transport property, stable electrode, easy process to form thin-film and helps to full coverage deposition of CBO. In addition to that, Cu-vacancies were created to improve the charge carrier concentration and facilitate the charge separation and transfer in the CBO photocathode. By changing the O₂ partial pressure, the density of Cu vacancies can be tuned, which leads to improved PEC performance. Introducing dopant to the NiO_x HTL and with copper-vacant CBO photocathode achieved a positive onset potential of ~1.22 V vs RHE and observed twofold improvement in photocurrent density. Prepared photoelectrodes optical and structural properties were examined well. This study offers new thoughtful for building progressed CBO photocathodes by thoroughly investigating photo-charge carrier separation and transfer with an improved photoelectrochemical performance of high-quality HTL and V_{Cu}-CBO photoelectrode for PEC water splitting reactions.



Poster Presentation : **PHYS.P-348**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Modification of the Electronic Transition by Varying the Composition of $\text{Cd}_x\text{Hg}_{1-x}\text{Se}$ Alloy Nanocrystals

Yoon Seo Jung, Kwang Seob Jeong*

Department of Chemistry, Korea University, Korea

Quantum dots have attracted much attention due to their bandgap tunability depending on the physical size. The physical properties of the QDs can be controlled by introducing impurities into the nanocrystals. Here, we present the $\text{Cd}_x\text{Hg}_{1-x}\text{Se}$ alloy nanocrystals which have a tunable electronic transition over a wide wavelength range. An addition of the Hg precursors into the CdSe CQDs causes the redshift of the major electronic transition in frequency from the visible to mid-IR range. Moreover, a gradual increase of the Hg^{2+} ratio results in the enhancement of the electron density, simultaneously leading to the appearance of the localized surface plasmon resonances (LSPRs) in the mid-IR region. Surprisingly, the Electron Paramagnetic Resonance (EPR) measurement shows that the singly-occupied quantum state (SOQS) can be observed during the synthesis of the $\text{Cd}_x\text{Hg}_{1-x}\text{Se}$ alloy NCs. The g-factor progressively shifts to the free electron signal as introducing more Hg^{2+} to the alloy. The intrinsic semiconductor property of CdSe can be shifted to the semi-metal property by increasing the Hg^{2+} doping concentration. Therefore, the $\text{Cd}_x\text{Hg}_{1-x}\text{Se}$ NCs are useful material to study the detailed electron dynamics when the semiconductor to semi-metal transition occurs in the NCs.

Poster Presentation : **PHYS.P-349**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Carbon dioxide reduction in the di-anionic state of nitrogen-containing PAH molecules

One Heo, Sang Hak Lee*

Department of Chemistry, Pusan National University, Korea

Nitrogen-doped graphene has been used as a catalyst to convert carbon dioxide molecules to useful chemicals such as methanol or ethanol through chemical reduction. In chemical reduction, the key step in the conversion is the reduction of carbon dioxide molecules that occurs when they are captured and the bond order reduced to weaken the bonding energy of the carbon dioxide. Previously, several studies have shown that nitrogen-containing PAH molecules have the catalytic property to convert carbon dioxide molecules in their anionic state. Nevertheless, in the anionic state, when nitrogen-containing PAH molecules have more than two nitrogen atoms, some of them invariably fail to interact with the carbon dioxide molecules. Thus, in this study, we investigated whether all nitrogen atoms in N-PAH molecules interact with carbon dioxide molecules in the dianionic state. When they are sufficiently negatively charged, N-PAH molecules have a stronger catalytic effect in the carbon dioxide reduction when in the di-anionic state than in the neutral or anionic states. More practically, we concluded that the optimal catalytic effect for carbon dioxide reduction occurs when the charge density of aza-naphthalene or -anthracene is higher than 1.7×10^{19} electrons/m², which is about 1 A/cm².

Poster Presentation : **PHYS.P-350**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Interaction Between Polyhexamethylene Guanidine (PHMG) and Lung Surfactant Membranes: Molecular Dynamics Simulation Studies

Jiyeon Hyun, Rakwoo Chang*

Department of Applied Chemistry, University of Seoul, Korea

The toxicity of polyhexamethylene guanidine (PHMG) and oligo (2-ethoxy) ethoxyethyl guanidinium chloride (PGH) used as humidifier disinfectants has recently been confirmed by the Korea Centers for Disease Control and Prevention (KCDC). It was found that they can cause pulmonary injury when inhaled. In this study, we have investigated the interaction between PHMG molecules and lung surfactant membranes consisting of dipalmitoylphosphatidylcholine (DPPC) monolayers using molecular dynamics simulations. Two types of PHMG molecules are used: bare PHMG and one in a water droplet mimicking aerosol. We have observed that the water droplet induces a water pore in the DPPC monolayer membrane, through which the PHMG molecule can enter the water phase. We have also investigated the effects of PHMG on neighboring DPPC lipids by calculating translational and orientational pair correlation functions.

Poster Presentation : **PHYS.P-351**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Catalytic Mechanism Study of Lactamase-like Esterase using Molecular Dynamics Simulation

YouHyun Nam, Rakwoo Chang*

Department of Applied Chemistry, University of Seoul, Korea

Penicillin-binding protein(PBP)/ β -lactamase(β L) homologs from *Pseudomonas fluorescens* (PfEstA), *Ruegeria Pomeroyi* (RpEstA), and *Caulobacter crescentus* (CcEstA) are esterases with β -lactamase activity. Previous experimental results showed that these three enzymes have the same catalytic residues(Serine, Lysine, and Tyrosine) with Class C β -Lactamase. Understanding the catalytic mechanism of these homologs will provide significant insights into this class of enzymes. Both ester and β -lactam catalyses of these PBP/ β L homologs have two steps: acylation and deacylation. In the acylation step, Ser acts as the nucleophile and Lys and Tyr as the general bases. To examine the expected conformation of catalytic triads and neighboring residues near the substrate during the acylation we ran Molecular Dynamics (MD) simulations of the *apo* conformation of these esterases in the presence of *p*-nitrophenyl acetate as the ester substrate. We have observed that in some cases the catalytic triads are not stable enough for the expected reaction to take place.

Poster Presentation : **PHYS.P-352**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Surface Structures and Electrochemical Behaviors of Self-Assembled Monolayers of Internally Functionalized Alkanethiols on Au(111)

Young Ji Son, Sichun Sung, TaeHo Yang, Jaegeun Noh*

Department of Chemistry, Hanyang University, Korea

Binding condition of molecule-metal interface and chemical structure of molecular backbone significantly affect the electronic properties of organic electronic devices such as organic light-emitting diodes (OLED), organic field-effect transistors (OFETs), organic memory, and solar cells. Particularly, self-assembled monolayers (SAMs) can solve the energy band alignment problems, which are frequently occurred in conventional materials such as conducting polymers and graphene, owing to their excellent chemical stability or functional manipulation. In this study, to understand the formation and structure of internally functionalized alkanethiol SAMs on Au(111), we prepared alkanethiol SAMs on Au (111) derived from aliphatic alkanethiol with an ester- or amide-functionalized alkyl chain. The surface structure and electrochemical behaviors of these SAMs were identified by using scanning tunneling microscopy (STM) and cyclic voltammetry (CV). 2-Mercaptoethyl heptanoate (2-MEH) SAMs formed line structures and gradually changed into disordered phases as the function of deposition time, while the surface structure of N-(2-mercaptoethyl)heptanamide (2-MEHA) SAMs was initially separated into two different phases, but as the formation time increases, most phases were composed of closely packed ordered structure. CV measurement showed that the reduction peaks of both functionalized alkanethiol SAMs were observed at less negative potentials of -974 mV for 2-MEH SAMs and -946 mV for 2-MEHA SAMs, compared to 1-decanethiol (DT) SAMs (-1115 mV). This can be ascribed to the presence of electro-withdrawing carbonyl group inside the alkyl chain, resulting in weakening the binding interactions between thiol and gold surface.

Poster Presentation : **PHYS.P-353**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Displacement Processes of Pre-adsorbed Octylamine Self-assembled Monolayers on Au (111) by Dodecanethiol

TaeHo Yang, Sichun Sung, Young Ji Son, Jaegun Noh*

Department of Chemistry, Hanyang University, Korea

Self-assembled monolayers (SAMs) are ultrathin films formed by spontaneous adsorption of organic molecules. They are especially appealing because of the ease of preparation and the variety of applications such as corrosion inhibition, molecular sensors, bio-interface, nanopatterning, and molecular electronics. In nanoparticle preparation, pre-capped alkyl-amine molecules are displaced by thiol ligands to functionalize the surface properties or to control the particle size. To understand molecular-scale displacement processes of alkylamine adsorbed on gold nanoparticles, we prepared pre-covered alkylamine monolayers on Au(111), which are subsequently displaced by alkyl thiols to form thiolate SAMs. In this study, we investigated the surface structure, binding condition, and reductive desorption of the monolayers before and after displacement of pre-adsorbed octylamine (OA) by dodecanethiol (DDT) using scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy and cyclic voltammetry (CV). STM measurements revealed that the octylamine SAMs with a disordered phase was changed to an ordered phase as a result of displacement by DDT. We also confirmed that the intensity of reductive desorption peak of OA SAMs at -960 mV decreased, whereas that of DDT SAMs at -1100 mV increased as function of displacement time.

Poster Presentation : **PHYS.P-354**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

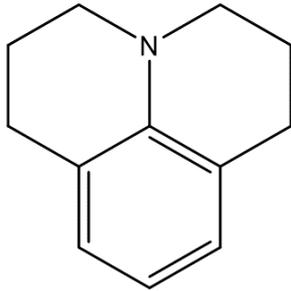
Why has N,N-Dimethylaniline been used as good donor on exciplex system?

Suhyun Park, Hohjai Lee*

Chemistry, Gwangju Institute of Science and Technology, Korea

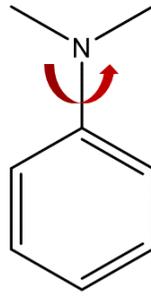
Exciplex is an emissive excited state complex of charged electron donor and acceptor formed after the photo-induced electron transfer. It has been studied for various fields such as OLEDs, light-emitting dye, magnetic field-sensitive fluorophore, etc. [1-2] However, it is not clear exactly what are the key molecular properties that allow exciplex formation. N,N-dimethylaniline (DMA) is a popular moiety as an exciplex-forming electron donor. Unlike DMA in which the C-N rotates freely, C-N rotation in julolidine (Jul) is constrained by the two six-membered rings, and it is known to be a more efficient electron donor than DMA due to its planar geometry, but a less efficient exciplex-forming electron donor. [3] On the other hand, for N,N-2,6-tetramethylaniline (TMA), the C-N rotation is sterically hindered to have a non-planar conformation. [4] In this poster I present the benefit of DMA as an exciplex-forming electron donor by the comparative spectroscopic studies with the Jul and TMA and DFT calculation from the view point of its molecular conformation. [1] *J. Mater. Chem. C.* 2019, 7, 11329[2] *J. Phys. Chem. Lett.* 2020, 11, 4668–4677[3] *J. Photochem. Photobiol. A.* 1996, 95, 127-136[4] *J. Phys. Chem.* 1991, 95, 2013-2021

Jul



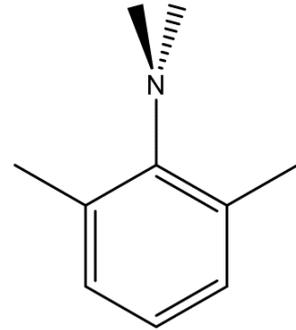
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DMA



$$0^\circ \leq \phi \leq 90^\circ$$

TMA



$$\phi \neq 0^\circ$$



Poster Presentation : **PHYS.P-355**

Physical Chemistry

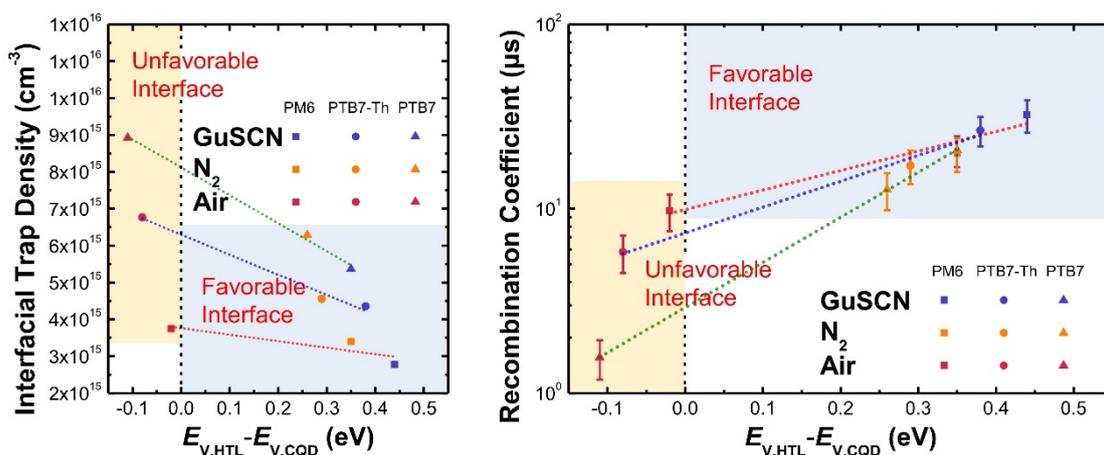
Zoom 9 FRI 15:00~16:00

Revisiting Energy Level Alignments at Colloidal Quantum Dot/Hole Transporter Interfaces toward Efficient Optoelectronics

Jonghee Yang, Whikun Yi*

Department of Chemistry, Hanyang University, Korea

Herein, we demonstrate a method to efficiently control the the energy levels of colloidal quantum dot (CQD) solids, particularly their Fermi level, as well as their p-/n-type characters. Additionally, we suggest that these features significantly affect to overall charge transport characteristics such as charge trapping, transfer, recombination and extraction. Our results, based on in-depth studies regarding carrier dynamics in devices, suggest that establishment of favorable interfacial energy level alignment, with a minimal interfacial carrier trap sites, markedly determines charge transport behavior and the performance of next-generation optoelectronics as a consequence.



Poster Presentation : **PHYS.P-356**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Composition- and Phase-Controlled Synthesis of Low-Dimensional Mo/Te Compounds by Te Flux Change

Hyeonkyeong Kim, Youngdong Yoo^{1,*}

Energy Systems Research, Ajou University, Korea

¹*Department of Chemistry, Ajou University, Korea*

Mo/Te compounds possess various electronic and optoelectronic properties depending on their composition and phase. In this study, we selectively synthesized 1D Mo₆Te₆ wires, and few-layer MoTe₂, and in-plane mixed-dimensional 1D-2D Mo₆Te₆-MoTe₂ heterostructures through chemical vapor deposition. The composition and phase of low-dimensional molybdenum/tellurium (Mo/Te) compounds are controlled by changing the Te atomic flux that is adjusted by the Te temperature. Under low Te flux, metallic 1D Mo₆Te₆ wire networks with 3-8 nm diameters and 100-300 nm lengths are obtained, whereas semiconducting few-layer 2H MoTe₂ films with 5-6 nm thick (8 layers) are synthesized with high Te flux. With medium Te flux, in-plane 1D-2D metal-semiconductor Mo₆Te₆-MoTe₂ heterostructures are formed. The synthesized 1D-2D Mo₆Te₆-MoTe₂ heterostructures are mixed-dimensional heterostructures with sharp interfaces between the 1D Mo₆Te₆ networks and the few-layer 2H MoTe₂ domains. The 2H MoTe₂ circular domains are edge-contacted by metallic 1D Mo₆Te₆. Raman mapping confirms that the 1D Mo₆Te₆ wire networks are first converted to mixed 1T'/2H MoTe₂ networks and finally to few-layer 2H MoTe₂ films by tellurization. The composition- and phase-controlled synthesis method through Te flux change could be utilized for large-scale fabrication of mixed-dimensional in-plane heterostructures and edge-contacted 2D electronic and optoelectronic devices.

Poster Presentation : **PHYS.P-357**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Photoexcitation dynamics of $[\text{Fe}(\text{NO})_2(\text{CysS}^-)_2]$ probed by time-resolved infrared spectroscopy

Woongsik Choi, Hojeong Yoon, Seongchul Park, Manho Lim*

Department of Chemistry, Pusan National University, Korea

Dinitrosyl iron complexes (DNIC) are known to play an important role in NO chemistry of mammalian biology. However, detailed reaction mechanism for the release of NO from DNIC and the bonding of NO has not been fully explored. Reaction of NO originated from DNIC can be probed by photodissociation of NO from DNIC. Photolysis of NO from $[\text{Fe}(\text{NO})_2(\text{CysS}^-)_2]$ was measured using time-resolved UV-Vis spectroscopy but the reaction dynamics was not obtained due to the difficulty in the assignment of the transient spectra to reaction intermediates. Here femtosecond time-resolved infrared spectroscopy will be used to investigate photoexcitation dynamics of $[\text{Fe}(\text{NO})_2(\text{CysS}^-)_2]$ in water after exciting at various wavelengths. $[\text{Fe}(\text{NO})_2(\text{CysS}^-)_2]$ was successively synthesized by properly mixing FeSO_4 , L-cysteine, and NO gas in D_2O . Equilibrium IR spectrum of $[\text{Fe}(\text{NO})_2(\text{CysS}^-)_2]$ displays two strong absorption bands at 1769 and 1719 cm^{-1} arising from asymmetric and symmetric NO stretching modes, respectively. Quantum chemical calculation shows that these bands shifts as CysS dissociates or one of them disappears as NO dissociates. Clear distinction for the reaction intermediates are expected. Detailed photoexcitation dynamics of $[\text{Fe}(\text{NO})_2(\text{CysS}^-)_2]$ and its implication in NO chemistry will be presented.

Poster Presentation : **PHYS.P-358**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Photoreaction Dynamics of Nitric Oxide from Cysteine like S-nitrosothiol

Manho Lim^{*}, Seongchul Park, Youjin Kim, Hojeong Yoon

Department of Chemistry, Pusan National University, Korea

S-nitrosothiol (RSNO), the most basic substance capable of providing nitric oxide, is a substance that is easily decomposed by heat and light. To create an environment similar to biological conditions, S-nitrosocysteine (CySNO) was synthesized by nitosation of Cysteine, a basic amino acid. However, CySNO has a relatively short lifetime, and S-nitroso-N-acetylcysteine (NacSNO), which is synthesized using N-acetylcysteine in which the amine group is substituted with amide, is used instead of cysteine, is a more stable material. In addition, S-nitroso-N-acetyl-penicillamine (SNAP), which is used as a basic model in many nitric oxide studies, is a molecule similar to NacSNO. We studied the photoreaction dynamics of RSNO made using Cysteine-like molecules. When all three molecules are exposed to light of 330 nm, they decompose at a rate faster than 0.3 ps to release NO, and some populations recombine in sub-ps. The non-recombinant population undergoes a bimolecular reaction with the surrounding RSNO to disulfide and generate RSSR. In particular, some populations have a special structure in CysSNO and NacSNO. As the C-S-N-O torsional angle becomes 90 degrees, it stabilizes, creates a torsionally relaxed structure, and returns to the ground state at a rate of several hundred ps. We can predict possible reactions when using RSNO as a NO donor through this study.

Poster Presentation : **PHYS.P-359**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

Photoexcitation dynamics of NO-bound cysteine

Youjin Kim, Hojeong Yoon, Seongchul Park, Manho Lim*

Department of Chemistry, Pusan National University, Korea

S-nitrosothiols (RSNO) have been studied as nitric oxide donors for decades. Decomposed nitric oxide has many biological functions, including platelet inactivation, immune suppression, neurotransmission, and vasodilation. S-Nitrosocysteine (CySNO) is known to play an important role in the delivery of NO in biological system. Completing the various reaction mechanisms that occur in the process of CySNO decomposing nitric oxide, is important information for use of CySNO in vivo or for interactions in surrounding biological systems. In this work, we probed photoexcitation dynamics of CySNO using femtosecond time-resolved infrared spectroscopy. The thermal lifetime of CySNO was probed by measuring the distinct electronic absorption of CySNO near 330 nm and the thermal stability of CySNO was optimized by adjusting pH and concentration. Excited CySNO by a 330-nm photon was found to rapidly photodissociate NO producing the CyS radical or transit to an electronically excited intermediate state. The portion of the nascent CyS radical geminated rebinds with NO or bimolecularly reacts with CySNO producing CySSCy and NO. The intermediate state relaxes into the ground state on the subnanosecond time scale. Biological implication of these reactions will be presented.

Poster Presentation : **PHYS.P-360**

Physical Chemistry

Zoom 9 FRI 15:00~16:00

The Mechanistic Study of 2-Ethyl-2-Adamantyl Chloroformate in Solvolysis

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The rates of 2-ethyl-2-adamantyl chloroformate was obtained in solvolysis, and it was analyzed by the extended Grunwald-Winstein equation ($\log(k/k_0) = lN_T + mY_{Cl} + c$). The calculated sensitivities for solvents both nucleophilicity and ionizing power were indicated to the unimolecular pathway like 1-adamantyl chloroformate, previously reported. This mechanism is contained the rate-determining step of ion pair of 2-ethyl-2-admantyl chloroformate in usual solvent system for solvolysis. These results were confronted with those of several alkyl chloroformates in order of the mechanistic comparison.

Poster Presentation : **PHYS.P-361**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Kinetics Study of H/D Exchange in the Alkylpyridinium Cation

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An alkylpyridinium ion is a cationic molecule in which an alkyl chain is attached to the nitrogen of a pyridine. Since there is no labile hydrogen such as acidic protons, hydrogen/deuterium exchange (HDX) is not much likely in the alkylpyridinium ion. However, previous studies showed the HDX of non-labile hydrogens at the pyridinium ring and proposed base-catalyzed mechanism which involves the carbanion formation. In the present work, we investigated detailed kinetics of HDX in the hexadecylpyridinium cation under the acidic and basic conditions using mass spectrometry (MS) and theoretical calculations. The numbers of exchanged hydrogens were counted by MS as a function of HDX reaction time and temperature, which were subsequently used to extract kinetic parameters such as the temperature-dependent reaction rate and the activation energy of HDX. As a result, HDX is much faster in the basic condition than in neutral or acidic conditions, which is in line with previous works suggesting base-catalyzed mechanisms. However, the determined activation energy is much lower than the predicted values for the HDX reaction with the carbanion formation. This suggests the presence of additional contribution of solvent and/or base molecules which decreases the activation energy of HDX at the pyridinium ring. Additional density functional theory calculations and experiments are on the way to find and verify a mechanism.

Poster Presentation : **PHYS.P-362**

Physical Chemistry

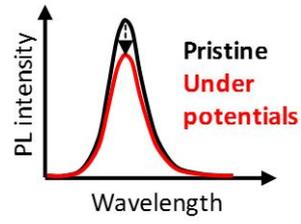
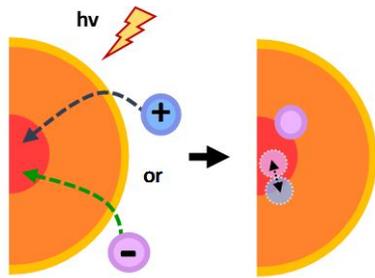
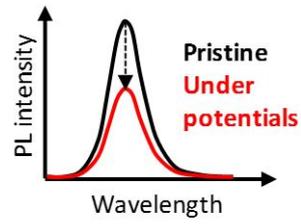
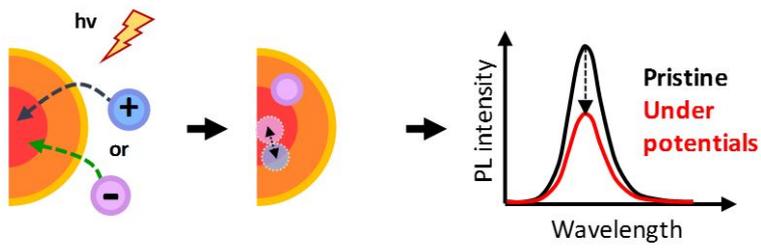
Zoom 9 FRI 16:00~17:00

Spectroelectrochemical Characterization of InP/ZnSe/ZnS Quantum Dots

Jumi Park, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Semiconductor quantum dot (QD) is spotlighted as a key emissive material for the next generation of light-emitting diodes (LEDs). This work presents the investigation of the electrochemical charging effect on the absorption and emission of the InP/ZnSe/ZnS QDs with different midshell thicknesses. The excitonic peak is gradually bleached during electrochemical charging, which is caused by $1S_e$ (or $1S_h$) state filling when the electron (or hole) was injected into the InP core. Additional charges also lead to photoluminescence (PL) intensity reduction, however, it is greatly mitigated as the midshell thickness increases. Various PL measurements reveal that the PL reduction under electrochemical charging is attributed to the acoustic phonon-assisted Auger recombination. Here, the Auger recombination in QDs with a thick midshell is reduced under the electrochemically charged condition, indicating that QDs with larger volume are more stable emitters in charge-injecting devices such as LEDs. Furthermore, the negative and positive trion Auger recombination rate constants are estimated, respectively, via electrochemical charging. The negative trion Auger rate constants decrease with an increase in the midshell thickness increases, whereas the positive trion Auger rate constants are not heavily reliant on the midshell thickness.



Suppressing Auger recombination in InP QDs with thicker midshell

Charged dot Auger recombination



Poster Presentation : **PHYS.P-363**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

A new drug-likeness score using negative data and LightGBM

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Identifying the characteristics of orally absorbable drugs are important for novel drug design. Previously, several empirical rules to discriminate druglike molecules from non-drug molecules such as Lipinski's rule of five and the QED score. Lipinski's rule is based on five molecular properties and the QED score is calculated using eight physicochemical properties of molecules that assumed to be important for quantification of newly created drugs. However, although the QED is derived from 771 approved drug, its discrimination power has not been extensively tested. Here we propose a new drug-likeness score, which distinguishes drugs from non-drug molecules. We trained a machine-learning-based score that discriminates 1169 approved drugs from non-drugs using fingerprints and various physicochemical properties using the LightGBM algorithm. We show that our score is more effective in discriminating drugs from non-drugs than QED. Our results suggest that considering negative cases is important in training an effective model.

Poster Presentation : **PHYS.P-364**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Comparing Compound I species with mono and fused di-porphyrin ligands using Density Functional Theory

Kyung-Bin Cho^{*}, Youngseob Lee¹

Department of Chemistry, Jeonbuk National University, Korea

¹*Chemistry, Jeonbuk National University, Korea*

It is now well known that heme enzymes like Cytochrome P450 uses a high-valent Fe(IV)O ligand radical cation system (so-called Compound I, Cpd I) to perform its oxidizing functions. Numerous experimental and theoretical studies have already been done to find out the exact reaction mechanistical details of such a reaction, and the details are by now quite clear, albeit some works remains. In this study, we are looking into using fused di-porphyrin systems using Density Functional Theory, to examine whether there are any differences to a monoporphyrin system. These di-porphyrin systems also contain Fe(IV)O cores in each of the porphyrin center, but there would now be two ligand cation radicals and distributed throughout this mega-complex, if the electronic structure would be exactly the same as in mono-porphyrin Cpd I, which does not seem to be likely. Hence, we are looking into the exact electronic configuration of this species and its reactivity, which may be regarded as emulating a metal-organic framework (MOF) in its simplest form.

Poster Presentation : **PHYS.P-365**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

The NMR Dynamics study of Transcription Factor protein DLX3 and DLX3-DNA complex.

Ho-seong Jin, Joon-Hwa Lee^{1,*}

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Transcription is carried out by an enzyme called RNA polymerase and a number of accessory proteins called transcription factors. Transcription factors(TF) can bind to specific DNA sequences called enhancer and promoter sequences in order to recruit RNA polymerase to an appropriate transcription site. The homeodomain transcription factor distal-less homeobox 3 gene (DLX3) is required for hair, tooth and skeletal development. DLX3 mutations have been found to be responsible for Tricho-Dento-Osseous(TDO) syndrome, characterized by kinky hair, thin-pitted enamel and increased bone density. For gene transcription to occur, transcription factors must bind to specific sequences of DNA. To understand the molecular mechanisms of specific DNA recognition of DLX3, we have performed ¹H/¹⁵N HSQC experiment and imino proton NMR experiments between TF and consensus TF Binding Site in DNA. The exchange rate constants of the imino protons for the wild type DNA, and TF-DNA complex were measured by using water magnetization experiment.

Poster Presentation : **PHYS.P-366**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

The NMR Study of DNA recognition of Transcription Factor MEIS1

Seo-Ree Choi, Joon-Hwa Lee*

Department of Chemistry, Gyeongsang National University, Korea

Transcription factors are proteins that bind specific sites or elements in regulatory regions of DNA, known as promoters or enhancers, where they control the transcription or expression of target genes. MEIS1 (myeloid ecotropic viral insertion site 1) is a viral integration site in murine myeloid leukemia cells. This gene encodes a homeobox protein belonging to the TALE ('three amino acid loop extension') family of homeodomain-containing proteins. TALE proteins are distinguished by the presence of three extra amino acids in the loop binding the first to the second alpha helix of the homeodomain. The highly conserved DNA-binding TALE proteins define the family and is responsible for specific recognition of a common sequence motif, [5'- TGACA- 3']. Further DNA-binding specificity within TALE family members is determined by adjacent DNA sequences and through the binding of additional transcriptional partners. In order to characterize the molecular recognition of DNA by MEIS1, we performed NMR experiments on MEIS1 complexed with 10-bp DNA duplex, d(AGCTGACAGC)/ d(GCTGTCAGCT), (wt-msDNA) and its mutants using NMR. We also studied the binding features of MEIS1 for both wild type and mutant DNAs characterized its target DNA recognition.

Poster Presentation : **PHYS.P-367**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Controlled Synthesis of Monolayer $\text{MoS}_{2(1-x)}\text{Se}_{2x}$ Alloys with Tuned Bandgaps by Flux-Controlled Chemical Vapor Deposition

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Monolayer transition metal dichalcogenide alloys are two-dimensional materials that can be utilized for various novel applications due to their interesting physicochemical properties. In particular, the bandgap of the monolayer transition metal dichalcogenide alloys can be tuned depending on their composition, which is very useful for electronic and optoelectronic applications. In this study, we report the controlled synthesis of monolayer $\text{MoS}_{2(x-1)}\text{Se}_{2x}$ alloys with tuned bandgaps through chemical vapor deposition. Depending on the S/Se ratio that is controlled by adjusting the temperature of S and Se, the bandgap of monolayer $\text{MoS}_{2(x-1)}\text{Se}_{2x}$ alloys is tuned in the range of 1.53 eV to 1.85 eV. We believe that as-synthesized monolayer $\text{MoS}_{2(x-1)}\text{Se}_{2x}$ alloys could serve as novel building blocks for various flexible optoelectronic devices.

Poster Presentation : **PHYS.P-368**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

DFT reaction mechanism study for the phenoxide migration at a Nickel(II) - tridentate bis(phosphenophenyl)phosphido ligand

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Recently, the $(P_2P-PP_2)\{Ni(CO)\}_2$ nickel (0) compound has been reported ($PPP- = -P[2-P^iPr_2C_6H_4]_2$) and its reaction with 2,4,6-tri-tert-butylphenoxy (OAr) radical produced $(PP^{OAr}P)Ni(CO)$.¹ The synthesis of $(PP^{OAr}P)Ni(CO)$ is also possible starting from the nickel (II) phenoxide compound $(PPP)NiOAr'$ with $OAr' = -OC_6H_4OCH_3, -OC_6H_4CH_3, -OC_6H_5, -OC_6H_4CF_3,$ and $-OC_6F_5$ in the presence of carbon monoxide. We studied the reaction mechanism for this process using DFT to explain how the change on OAr' affected the speed of the reaction. The process was studied considering the closed shell and open shell options. The $S = 1$ state of $(PPP)NiOAr'$ exhibits spin accumulation on the central P atom of PPP and no significant spin density on OAr' in several steps of the mechanism. This is consistent with previous reports of the PPP ligand.² We also identified the Ni- OAr' break as a crucial step for this mechanism. *Corresponding authors †Jeonbuk National University ‡ Seoul National University 1.Y.-E. Kim and Y. Lee, *Angewandte Chemie International Edition*, 2018, 57, 14159-14163. 2.Y. M. Rhee and M. Head-Gordon, *Journal of the American Chemical Society*, 2008, 130, 3878-3887.

Poster Presentation : **PHYS.P-369**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Selective Depletion of Stimulated Raman Scattering of Rhodamine Dyes with Two Strong Raman-active Modes

Jaeyoon Lee, Sang-Hee Shim*

Department of Chemistry, Korea University, Korea

Stimulated Raman scattering (SRS) microscopy is an emerging imaging modalities for biological systems. The narrow spectral bandwidths and resistance to photobleaching complement the shortcomings of fluorescence microscopy. However, optical diffraction limits the spatial resolution. Selective suppression of SRS by another competing SRS was proposed as a plausible option for diffraction-unlimited SRS microscopy. In this scheme, the depletion efficiency and spatial resolution depend on the Raman cross-sections of the two competing Raman-active modes. To maximize the resolution enhancement effect, we performed three-beam SRS experiments of Rhodamine dyes with a nitrile or alkyne group as an additional Raman-active probe in the cell-free window. For the detection mode, we used the vibrational mode of conjugated double bonds at ~ 1600 cm^{-1} whose SRS intensity is amplified by electronic pre-resonance. Also, the vibrational mode of nitrile or alkyne group at 2100-2200 cm^{-1} with strong Raman cross-sections was used for depleting the SRS of the double-bond mode. We obtained up to 80% efficiency for the depletion of SR gain of the double-bond mode in Rhodamine 800 dye by the nitrile stretch mode with the maximum depletion intensity of 0.75 TW/ cm^2 at 1030 nm. From series of dyes with various Raman cross-sections for the detection and depletion modes, we investigate how the Raman cross-sections and electronic pre-resonance conditions play roles in the depletion efficiencies and the spatial resolutions.

Poster Presentation : **PHYS.P-370**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Investigation of Electron Transport through π -Conjugated Molecular Bridge in Si QD Dimer Using NEGF Method

Jiyoung Bang, Young-Hwa Choi¹, Hyun-Dam Jeong^{1,*}

Department of chemistry, Chonnam National University, Korea

¹Department of Chemistry, Chonnam National University, Korea

Silicon quantum dot (Si QD) clusters can be applied to thermoelectric materials and LIB anode materials that require high electron transport properties. The electron transport properties of the Si QD clusters can be controlled by molecular bridges. We calculated electron transport properties in a Si QD dimer system linked by π -conjugated molecular bridges to speculate the electron transport properties of its relevant Si QD clusters. The effects of the bond order in π -conjugated molecular bridges on their electron transport properties were investigated with the NEGF method using MATLAB, where two vinylenes terminating the two Si QDs are connected each other by single, double, and triple bonds, respectively. Furthermore, this kind of calculation was also performed even for the gold electrode system consisting of gold clusters to investigate the effect of the kind of electrode on the electron transport properties. With the Si QD cluster electrodes, the current for the double bond is greater than that for the triple bond, while, in the Au cluster electrodes, the electron transport properties through molecules raise with increasing their bond order.

Poster Presentation : **PHYS.P-371**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Development of electron beam lithography photoresist based on In₂O₃ nanocrystals

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

With the development of the semiconductor industry and the increasing demand for highly integrated devices, the development of next-generation lithography technology for device manufacturing is underway. Electronic beam lithography (EBL) is known as one of the next generation lithography technologies, which is the only technology without using mask, and, accordingly, the development of resists for electron beam lithography needs to be carried out. We focused on inorganic resist because it has advantages such as better etch resistance and contrast over traditional organic resist. Indium oxide nanocrystal (In₂O₃ NC) was synthesized using oleic acid (OA) by hot injection method. In order to investigate the change in photoresist properties according to the difference of the ligand molecule, the ligand exchange reaction between OA-capped In₂O₃ NC and benzoic acid (BA) and 4-aminobenzoic acid (4ABA) was performed to synthesize BA-capped In₂O₃ NC and 4ABA-capped In₂O₃ NC. Dissolution contrast curves for the three NC thin films was obtained and compared each other.

Poster Presentation : **PHYS.P-372**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Artificial Mass Spectra Generation with Transformer

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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 are used for compound identification in the absence of a commercial standard reference spectrum. Reference libraries provide fast and reliable identification for compounds whose fragmentation patterns are revealed. However, the limited coverage of available reference libraries has led to an interest in machine learning models for predicting mass spectra from chemical structures. In this report, we propose a direct translation approach for mass spectra prediction from molecular fingerprints. We show that a neural machine translation approach with Transformer architecture can be used effectively to predict mass spectra from its molecular fingerprint or vice versa. We manage to generate high-quality mass spectra data based on the cosine and Tanimoto similarity metric assessments. This proposed approach has high potential for broad applications in the chemical analysis of unknown substances.

Poster Presentation : **PHYS.P-373**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Investigation of Organic Ligand and Curing Temperature Dependence on the Electronic Structure of Indium Oxide Nanocrystal Thin Film Using Energy-Resolved Electrochemical Impedance Spectroscopy and Cyclic Voltammetry

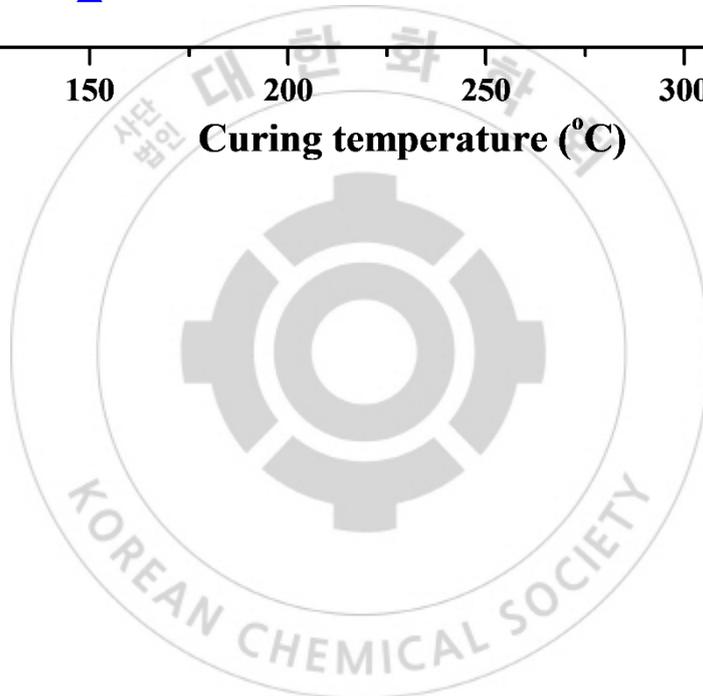
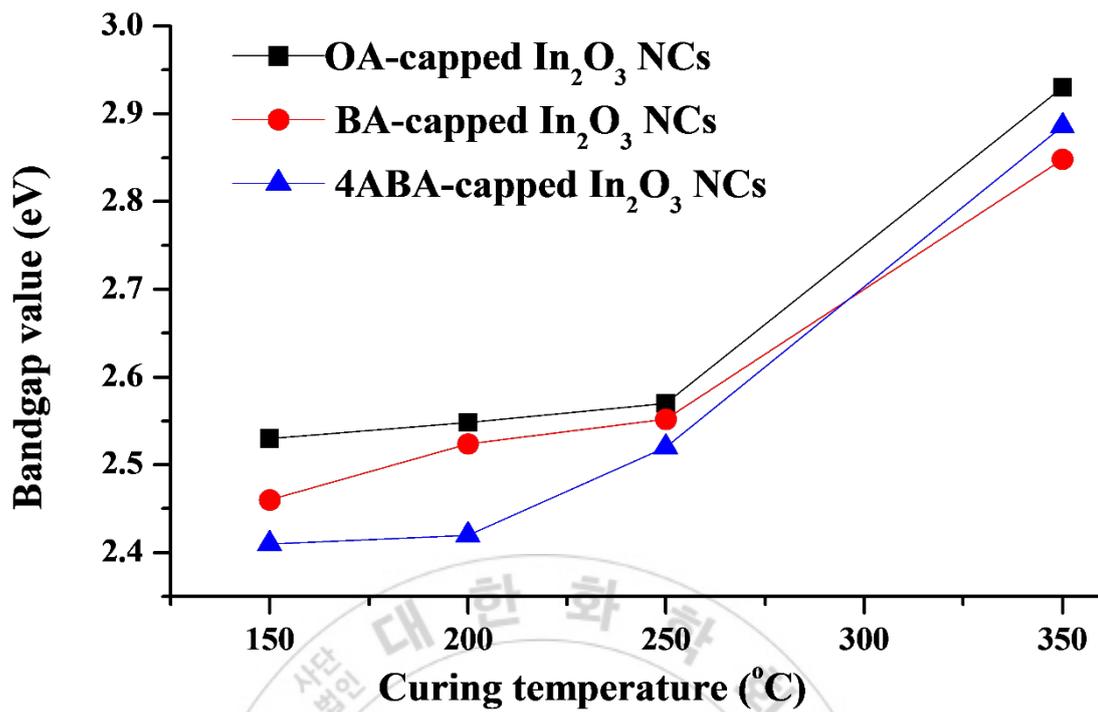
Quang Trung Le, Hyeonbeom Park¹, Hyun-Dam Jeong^{2,*}

Chonnam National University, Vietnam

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²*Department of Chemistry, Chonnam National University, Korea*

We investigated the dependence of organic ligands and curing temperature on the electronic structure of indium oxide nanocrystal (In_2O_3 NC) thin film using energy-resolved electrochemical impedance spectroscopy (ER-EIS) and cyclic voltammetry (CV) method. In_2O_3 NC capped with various organic ligands, namely oleic acid (OA), benzoic acid (BA), and 4-amino benzoic acid (4ABA) were prepared by hot-injection method and ligand exchange reaction. The electrodes for EIS and CV measurements were fabricated by spin-coating with a solution of In_2O_3 NC capped with various organic ligands on an ITO substrate. The electronic structure of In_2O_3 NC capped with OA, BA, and 4ABA thin films cured at 150, 200, 250, 350 degrees were quantified by ER-EIS and CV measurement. The bandgap value of In_2O_3 NC-based thin film increased with increasing the length of the organic ligand and the curing temperature. Based on thermogravimetric analysis spectra, we also identified the temperature range at which organic ligand molecules still exist on the surface of In_2O_3 NC. The electron mobility of the BA-capped In_2O_3 NC and 4ABA-capped In_2O_3 NC thin films increases significantly as compared with that for OA-capped In_2O_3 NC thin film. Especially, in case of curing at 200°C, the activation energy and electronic coupling for electron transfer between the adjacent NCs in the In_2O_3 NC thin films is estimated, based on Marcus theory, by using the temperature dependence of electron mobility on their thin film transistors (TFTs).



Poster Presentation : **PHYS.P-374**

Physical Chemistry

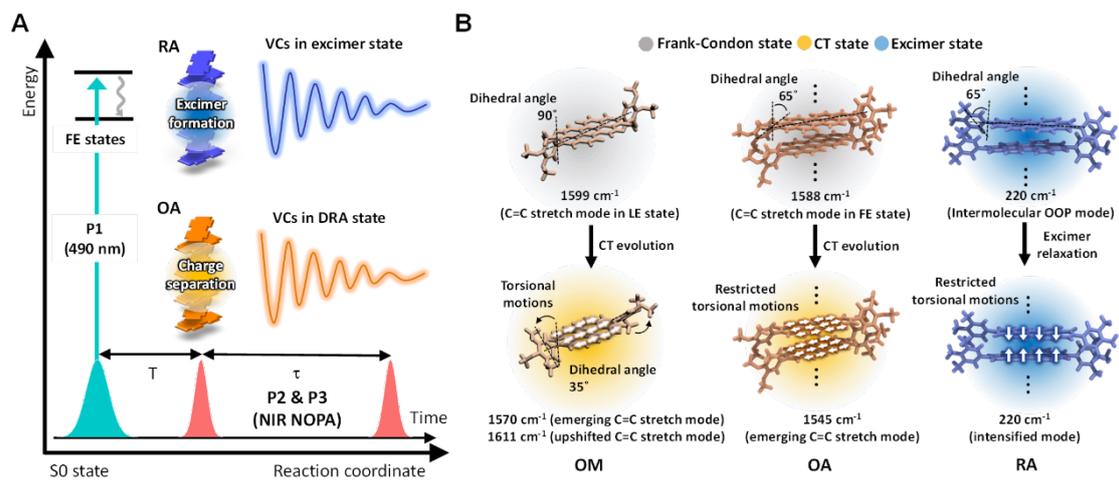
Zoom 9 FRI 16:00~17:00

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-375**

Physical Chemistry

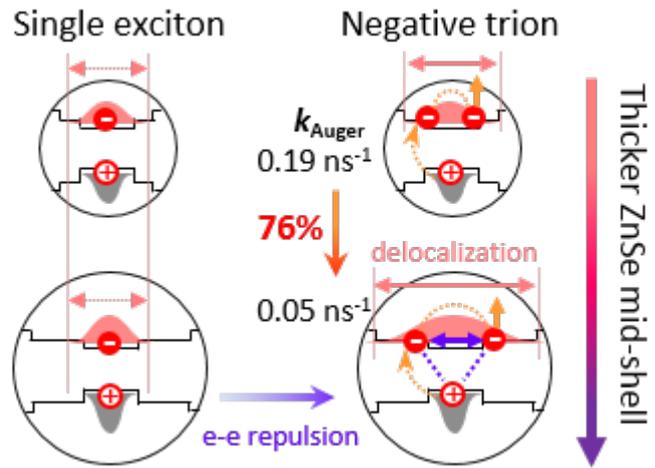
Zoom 9 FRI 16:00~17:00

Negative Trion Auger Recombination in InP/ZnSe/ZnS Quantum Dots

Taehee Kim, Dongho Kim*

Department of Chemistry, Yonsei University, Korea

Eco-friendly quantum dots (QDs) are recently in the spotlight for the light emitting materials applicable to the commercial display products. Upon demonstrating the quantum dot based light emitting devices (QD-LEDs), the rapid nonradiative Auger recombination process acts as one of the main performance limiting factors. Recent advances in nontoxic QD-LED performance by QD shell engineering have thus inspired us to investigate the Auger-related photophysics in relation with the variously tuned QD nanostructures. Here, we report the negative trion Auger recombination of highly luminescent InP/ZnSe/ZnS QDs with different mid-shell structures that affect the performances of QD-LEDs. Transient PL measurements reveal that exciton-exciton binding energy depends on the mid-shell thickness, which implies that the intercarrier Coulomb interaction caused by the introduction of excess charges may come under the influence of mid-shell thickness, in contrast with the nearly stationary single exciton behavior. We employed photochemical electron-doping on colloidal QD ensemble to directly generate the negative trion species. Moreover, by monitoring the single QD charging the negative trion behavior could also be analyzed. Both the ensemble and single dot measurements showed that negative trion Auger recombination exhibits strong dependence on mid-shell thickness. This was further supported by the dynamics of hot electron generated directly in ZnSe mid-shell. These results highlight the role of excess electrons and the effects of engineered shell structures in InP/ZnSe/ZnS QDs, which eventually determine the Auger recombination and QD-LED performances.



Poster Presentation : **PHYS.P-376**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Long-range corrected density functional theory study on the effect of end-capped electron withdrawing group in conjugated polyene on charge transfer excitation energy

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We performed intra-molecular charge transfer (CT) excitation energy calculations of conjugated carbon chain [H₂N-(C=C)_n-X: n=2~8] with various functional groups (X= NH₂, OH, Cl, CHO, CN, and NO₂) using EOM-CCSD, time-dependent (TD) HF, and various TD density functional theory (DFT), such as BLYP, B3LYP, long-range corrected (LC) DFT in order to analyze the effect of electron withdrawing (or donating) strength of end-capped functional group on CT excitation energy. Additionally, we performed inter-molecular CT excitation energy calculations of inter-molecular systems of H₂NH...HX which have identical distances with fore-mentioned H₂N-(C=C)_n-X (n=2~8) to analyze the effect of electron withdrawing (or donating) strength of end-capped functional group on inter-molecular CT excitation energy. We found that in both inter- and intra-molecular cases LC-BLYP functional with the default range-separation parameter showed the closest CT excitation energies to EOM-CCSD ones. According to distance between two functional groups, intra-molecular CT excitation energy decreases, but inter-molecular CT excitation energy increases. This is because the electron withdrawing group induces LUMO energy decreasing, which decreases the HOMO-LUMO gap. Overall, as electron withdrawing strength increases, CT excitation energy tends to decrease in both intra- and inter-molecular systems. However, in case of intra-molecular CT excitation energy, the effect of electron withdrawing group is negligibly small (at most 0.5 eV) in intra-molecular CT excitation energy. Noticeably, we found that cyano group (-CN), which is known as strong electron withdrawing group, unexpectedly increases LUMO energy, which results in large HOMO-LUMO gap and large CT excitation energy in inter-molecular cases.

Poster Presentation : **PHYS.P-377**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Effect of Entropic Interaction between Polymer-Tethered Nanoparticles and Block Copolymers on Their Assembly within Emulsion

Meng Xu, Bumjoon Kim*

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The assembly of hybrid materials with well-defined morphologies is important to design complex nanomaterials. Here we show a design of entropy-driven particle assemblies with polystyrene-grafted Au nanoparticles (Au@PS) within onion-like polystyrene-*b*-poly(4-vinyl pyridine) (PS-*b*-P4VP) block copolymer (BCP) particles. We observed transitions of hybrid particles between alternate-layered onions, seeded onions, and crusted onions by tuning four parameters: molecular weight (N) and grafting density of PS ligands, core size of Au@PS, and M_n of PS blocks (P). To account for the phenomena, a modified swelling ratio (P/N_{SDPB}) is proposed by considering the ligands in semi-dilute polymer brush (SDPB) regime as the only brushes available for interfacial interactions with BCPs. The modified parameter successfully explains structural transitions.

Poster Presentation : **PHYS.P-378**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

First-principles Investigations of Reaction Mechanisms of Tetrakis (ethylmethylamino) Hafnium – Water Atomic Layer Deposition Process

Hyeyoung Shin

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The hafnium oxide (HfO₂) has attracted much attention due to its high permittivity, wide bandgap and thermal and chemical stabilities. The HfO₂ atomic layer deposition (ALD) using tetrakis(ethylmethylamino) hafnium (TEMAH) and water on the partially hydroxylated Si(100) surface is investigated using periodic dispersion corrected DFT calculations. Chemisorption of TEMAH on the Si(100) surface occurs through first ligand-exchange reaction which forms tri(ethylmethylamino) hafnium and releases one ethylmethylamine molecule. The energies of possible reaction pathways suggested that mono(ethylmethylamino) hafnium is found as final product in the precursor pulse. The ligand-exchange reaction between water and mono(ethylmethylamino) hafnium in the water pulse results in unsaturated hafnium. The research gives us better understanding about how the first HfO₂ layer is formed on the partially hydroxylated Si(100) surface.

Poster Presentation : **PHYS.P-379**

Physical Chemistry

Zoom 9 FRI 16:00~17:00

Two Dimensional ZnIn₂S₄ Nanosheets Wrapped Blue TiO₂ Nanorods for Photocatalytic Reduction of CO₂ into Solar Fuels

Praveen kumar Dharani, Tae Kyu Kim*

Department of Chemistry, Yonsei University, Korea

Development of noble metal free, novel and highly efficient photocatalyst is of great significance in favor of high performance and selective photocatalytic CO₂ conversion. The present existing technologies for photocatalytic CO₂ conversion primarily involves the use of noble metals as co-catalysts on semiconductor materials resulting in significantly improved photocatalytic CO₂ reduction. However, because of the high cost and low abundance of noble metals, its practical use is limited. In this study, noble metal free heterostructures of blue TiO₂ nanorods (BT) and hexagonal ZnIn₂S₄ (ZIS) nanosheets are fabricated. The BT has higher electron mobility and specific surface area, moreover, it has bandgap around 2.8 eV that reduces recombination of electron-hole pair owing to quantum confinement effect. In the same way ZIS has low bandgap material for effective absorption of visible light. Band structure of BT/ZIS composite is proved by Mott Schottky measurement and diffuse reflectance spectroscopy. In this mechanism, photogenerated electrons in the conduction band of ZIS are moving to that of BT, which reduces CO₂ to CO by being oxidized to the original state simultaneously. 6 wt% BT/ZIS composite shows radically higher CO production than BT and ZIS respectively. It produces CO with the rate of 70 μmol g⁻¹ h⁻¹, which is 2.6 times faster than CO production rate of ZIS. The stability of this material is proved by the long-time experiment. BT/ZIS heterostructure has a fine duration under solar light irradiation for about 7 days. This was also shown by 5 times of recycling test, showing almost same activity and selectivity during this experiment

Poster Presentation : **ANAL.P-380**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Clustering and dehydration of lactic acid

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Lactic acid is a substance mainly present in human sweat. It has been utilized in the food and pharmaceutical industries. Due to the demand for lactic acid bacteria, synthesis of lactic acid was required. It is reported that 68,000 tons of lactic acid are produced every year until 2006. Also, the market growth rate of lactic acid is expected to be 10% to 15% per year. Liquid chromatography is generally used to analyze lactic acid in extracts of fruits and grains or in blood lactic acid concentration analysis. UV detectors are often used for lactic acid, but the purity of commercially available lactic acid is generally less than 90%. Since methanol, ethanol, acetic acid, and pyruvic acid are present as impurities, the standard for lactic acid is difficult to determine. A method that can be analyzed without a standard is a mass spectrometric technique. Atmospheric pressure chemical ionization (APCI) is a weak ionization method that ionizes an analyte from an ionized solvent. Lactic acid has a property of forming clusters and dehydration at high temperature and high pressure. In this study, the behaviors of clustering and dehydration of lactic acid were investigated by varying the source fragmentor voltage and heating temperature.

Poster Presentation : **ANAL.P-381**

Analytical Chemistry

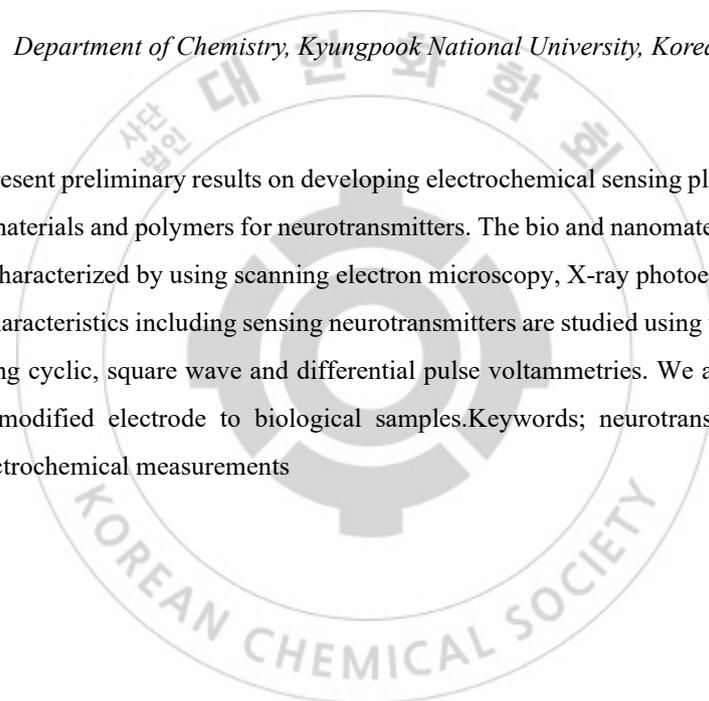
Zoom 10 FRI 15:00~16:00

Electrochemical sensing platform integrating nano and bio materials for neurotransmitters

Jingjing Li, Hye Jin Lee*

Department of Chemistry, Kyungpook National University, Korea

In this poster we present preliminary results on developing electrochemical sensing platforms with metallic nanoparticles, biomaterials and polymers for neurotransmitters. The bio and nanomaterials on the electrode surface were characterized by using scanning electron microscopy, X-ray photoelectron spectroscopy. Electrochemical characteristics including sensing neurotransmitters are studied using various voltammetric techniques including cyclic, square wave and differential pulse voltammetries. We also applied our nano and bio material modified electrode to biological samples. Keywords; neurotransmitter, biomaterials, nanomaterials, electrochemical measurements



Poster Presentation : **ANAL.P-382**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Development of an universal method for simultaneous analysis of 46 neurotransmitters in mouse brain cell culture medium, tissue lysate and serum using liquid chromatography coupled to tandem mass spectrometry

Nu Ri Lim, Ki Hun Kim*

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Neurotransmitters play an important physiological role in the body, which have been associated with diseases. Therefore, accurate measurement of neurotransmitters in diverse matrices is essential as it can provide a procedure for diagnosing and treating diseases. In this study, we developed and optimized the rapid simultaneous analytical method for multiple neurotransmitters remaining in fetal mouse brain cell culture medium, brain tissue lysate and mouse serum using liquid chromatography coupled to tandem mass spectrometry. We optimized analytical methods for 46 target neurotransmitters and their metabolites to improve the reproducibility and accuracy of the benzoyl chloride derivatization preparation process. We focused to optimized benzoyl chloride concentration, derivatization temperature and reaction time for high sensitivity and the values were that 0.5%, 1 °C and 10 minutes, respectively. Furthermore, pH (9.6 with carbonate-bicarbonate buffer) was also critical factor, and we observed an increase in sensitivity for Adenosine (684.7%), 3-methoxytyramine (112.6%), Spermidine (72.5%), Serotonin (41.1%), Tyramine (57.0%), Dopamine (35.3%) and Epinephrine (22.5%) compared to using sodium carbonate solution. The method with derivatization of samples was validated. Linearity was obtained ($R^2 \geq 0.98$) and the intra and inter-day precision of the method were ranged from 9.6% to 24.0%. The accuracy of the method was 85.0~114.6%. The developed method could be suitable for rapid analyzing neurotransmitters in various matrices.

Poster Presentation : **ANAL.P-383**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Effective Sample Preparation and determination of nicotine enantiomer in E-Liquid using Dispersive Liquid-Liquid Microextraction HPLC-UV

Seung Hoon Song, Seung Woon Myung*

Department of Chemistry, Kyonggi University, Korea

In this study, the contents of (S)-(-)-nicotine and (R)-(+)-nicotine were analyzed for various types of nicotine after efficiently extract the enantiomeric nicotine present in E-Liquid using dispersive liquid-liquid microextraction(DLLME). In order to optimize DLLME, experiments were conducted on the pH, extraction solvent, dispersive solvent, and type and amount of salt. The LOD of chiral nicotine was 0.11 $\mu\text{g/mL}$ and 0.17 $\mu\text{g/mL}$, respectively, and the LOQ was 0.3 $\mu\text{g/mL}$, 0.44 $\mu\text{g/mL}$. It was confirmed through an experiment. The calibration curve was designed to be 0.3 – 18 $\mu\text{g/mL}$, 0.44 – 4.4 $\mu\text{g/mL}$, respectively, and the correlation coefficient (r^2) was 0.9978 – 0.9996. As a verification of the optimized method, accuracy and precision were measured by dividing it into intra-day and inter-day. In the experiment conducted with intra-day, accuracy was 79.9-110.6%, and the precision was 1.3-12.0%. In the inter-day, accuracy was 87.8 – 108.0%, and the precision was 4.0 – 12.8%. This analysis of chiral nicotine using DLLME uses less organic solvents than LLE method and is an excellent method that allows sample preparation within a short time.

Poster Presentation : **ANAL.P-384**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Comparing the properties of keratin from hair cortex and cuticle

Jungwoo Suh, Kwanwoo Shin*

Department of Chemistry, Sogang University, Korea

The human hair shaft consists of several layers. The two largest of these layers are the cortex and cuticle. Both two layers have keratin as their main component. However, their structure and function are quite different. Cortex comprises the main bulk with a fiber bundle structure, while the cuticle protects the interior with a stacked scale structure. We noted these aspects and determined that the keratin from each layer also would be different. To figure out the difference, we separated the cortex and cuticle with the blender and extracted the keratin from each layer, respectively. Keratin samples are analyzed via XRD to find the local difference in protein structure. Furthermore, keratin films are made in several different ways and exposed to an acidic environment. The composition and change caused by acid were analyzed with FT-IR. Keywords: cortex, cuticle, keratin

Poster Presentation : **ANAL.P-385**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Analytical Limitation of optical redox ratio in medical diagnosis

SooYeong Lim, Jin IL Jang, Chan Ryang Park, Hyung Min Kim*

Department of Chemistry, Kookmin University, Korea

Histopathology, which is the main method to diagnose cancer of patients, requires significant time because of histological staining process. In recent years, studies have been reported to reduce the time for histopathology. Among them, optical methods like autofluorescence imaging have witnessed remarkable progress, providing fast and endoscopic diagnosis. Autofluorescence spectra includes multiple origins such as connective tissues (collagen, elastin, keratin, etc.), porphyrins-series, NADH, and FAD. And there are many studies that optical redox ratio (ORR) is defined as the fluorescence intensity ratio between NADH and FAD and normal and cancer tissues are classified based on the ORR. However, there have been few reports that evaluate the accuracy of ORR based diagnosis. In this study, we prepared mixture of NADH and FAD in three different buffers and measured the time-dependent variation of ORR to measure in vitro evaluation of ORR reproducibility. The ORR was calculated by deconvoluting the of autofluorescence intensity of mixture solution with respect to NADH and FAD pure fluorescence spectra. We found that the experimental ORR had a linear relation with the calculated value from NADH and FAD concentration at that time they were prepared. However, this linear relationship changes over time and is maintained for only up to 2 days. We concluded that the ORR deviation from calculation resulted from the decrease in the fluorescence intensity of NADH over time, and it was confirmed in the UV absorption spectrum. In addition, we also tested the ORR variation depending on the buffer containing samples to evaluate the reproducibility. Consequently, it is suggested that the ORR ratio measurements should be performed within 2-3 days to provide accurate values in vitro condition.

Poster Presentation : **ANAL.P-386**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Development of analysis of HIF stabilizers in human urine for anti-doping by QuEChERS method and liquid chromatography-mass spectrometry

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Hypoxia-Inducible Factor Stabilizers (HIF stabilizers) are recently added prohibited drugs by the World Anti-Doping Agency, and they are considered to potentially improve athletes' athletic performance by activating genes associated with hypoxic reactions to increase the capacity of transporting oxygen. HIF stabilizers are difficult to analyze due to their unique structure and properties in liquid chromatography-mass spectrometry (LC-MS) using a reverse-phase column. In addition, it is necessary to apply a complementary sample preparation method rather than using only the solid phase extraction method to prevent false-positive results. In this study, we applied and optimized the QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) method as sample preparation for HIF stabilizers in human urine, and optimized the separation conditions for LC-MS. We optimized conditions for extraction solvent volume, number of extraction, and extraction pH for high efficiency. The final conditions are twice extraction with 1 mL of 1% formic acid (pH 3.2) in ACN. Separation efficiency and sensitivity of LC-MS were also improved by adjusting the mobile phase to 0.2% formic acid in water and 0.2% formic acid in ACN. The developed method was also validated for characteristics such as the limit of detection, matrix effect, recovery, and precision according to ISO17025 guidelines. LOD ranged from 0.1 to 1.0 ng/mL, 8.0 to 52.7% for matrix effect, 73.2 to 102.2% for recovery, 6.2 to 28.1% for intra-day precision, and 7.3 to 32.0% for inter-day precision. This study was firstly introduced for anti-doping analysis, and the developed method could be a complementary method for HIF stabilizers.

Poster Presentation : **ANAL.P-387**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Searching for novel organophosphate modification sites using high resolution mass spectrometry

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¹*Department of New Biology, DGIST, Korea*

Organophosphate compounds exhibit neurotoxicity by binding to the serine site of acetylcholinesterase (AChE) in the cholinergic nervous system and subsequently lead to the accumulation of acetylcholine. Butyrylcholinesterase (BchE) is known to play a similar role to AChE due to its ability to hydrolyze choline esters and the binding of organophosphate to blood BchE in patients with poisoning has been reported (Bin Li et al 2010). Since organophosphates are transported in blood vessels to modify serum albumin, studies have been carried out to search modification sites by organophosphates in human serum albumin (HSA), one of high abundant proteins in blood. Even though the reaction between HSA and organophosphate is considered to be slow compared to that with cholinesterase enzymes, the high abundance of HSA makes modified sites on HSA diagnostic signature. Therefore, modified sites on BchE and HSA are best examples to search for evidence of poisoning with organophosphates. In this study, BchE and HSA were treated with chemical models of organophosphate compounds. The peptides were prepared through tryptic digestion after quenching residual activity of the highly reactive chemicals, desalted by C18 cleanup cartridge, and analyzed by high resolution mass spectrometry online connected to nanoflow liquid chromatography system. The mass spectrometry data were analyzed using the MaxQuant platform (ver 1.6.15) by configuring specific modifications by the model chemicals. The result will be discussed in poster.

Poster Presentation : **ANAL.P-388**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Determining rotation angle of single anisotropic plasmonic nanoparticle using absorbance/scattering signals

Sungyeon Moon, Seong Ho Kang*

Department of Applied Chemistry, Kyung Hee University, Korea

Gold nanorod (AuNR), an anisotropic plasmonic nanoparticle, is a promising nanoparticle because it exhibits plasmon resonance when illuminated by light. AuNR has different optical properties depending on the direction. Herein, we observed the rotation angle of AuNR using light absorbance property in interference and light scattering property in total internal reflection. Differential interference contrast (DIC) microscopy utilized the optical path difference between two polarized lights as they passed through the AuNR. The phase delay of lights caused high contrast rendition of gradients and made the image like three-dimensional. By the DIC microscopy, the rotational mode of AuNR by deriving angle-dependent DIC image pattern could be resolved. The results were compared to the angle detection of AuNR by total internal reflection scattering microscopy to check the application of various types of microscopy according to the characteristics of the AuNR.

Poster Presentation : **ANAL.P-389**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

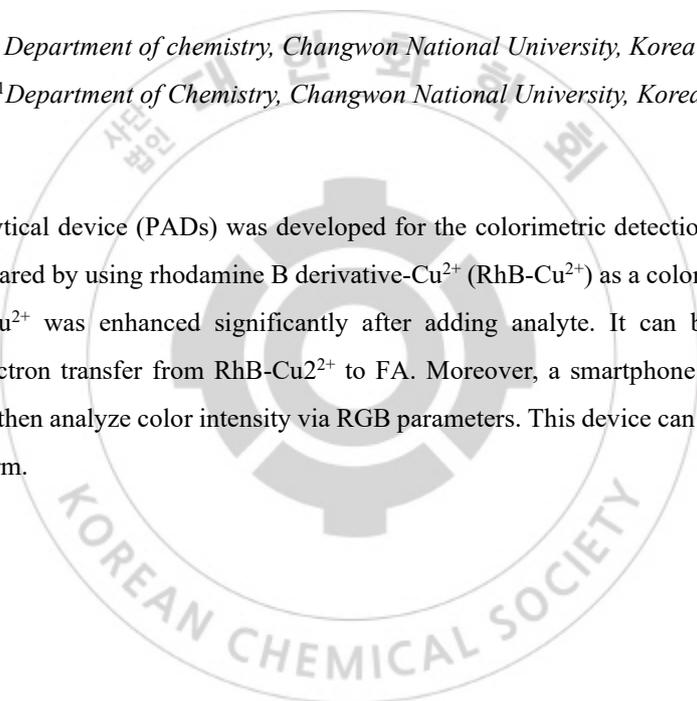
Rapid and visual detection of folic acid using paper-based analytical devices

DaeHyun Kwon, Nguyen Ngoc Nghia¹, Bui The Huy¹, Yong-Il Lee^{1,*}

Department of chemistry, Changwon National University, Korea

¹*Department of Chemistry, 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-Cu²⁺ (RhB-Cu²⁺) as a color indicator. The color intensity of RhB-Cu²⁺ was enhanced significantly after adding analyte. It can be explained by the improvement of electron transfer from RhB-Cu²⁺ 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-390**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Inkjet-based microreactor for the synthesis of silver nanoparticles on plasmonic paper decorated with chitosan nano-wrinkles for efficient on-site surface-enhanced Raman scattering (SERS)

Truong Thi thuy, Sharipov Mirkomil¹, Bui The Huy¹, Yong-Il Lee^{1,*}

chemistry, Changwon National University, Korea

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Here we report a synthesis approach that is simple, surfactant free, and green, and which is additionally cost effective in terms of its material requirements. The approach entails the use of an inkjet microreactor for the deposition of silver nanoparticles on the surface of office paper decorated with chitosan nano-wrinkles for the preparation of a reproducible and sensitive paper-based surface-enhanced Raman scattering (SERS) 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 (AA). Pre-modification of the paper with chitosan allowed the formation of randomly oriented nano-wrinkles on the surface, thus enabling the formation of silver nanoparticles with good hotspots. The novel paper-based SERS substrate showed outstanding sensitivity and spot-to-spot reproducibility for on-site detection using a portable Raman spectrometer with a limit of detection (LOD) of 10.7 pM. Moreover, our paper-based SERS substrate has an excellent enhancement factor (EF) of 7.4×10^8 , which is difficult to achieve on a paper substrate because of the microporous nature of paper. Finally, the batch-to-batch reproducibility and long-term stability of the SERS substrate under ambient conditions make this substrate a good candidate for point-of-care test (POCT) applications.

Poster Presentation : **ANAL.P-391**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Single Particle Study: Plasmonic Damping Induced by Mercury Amalgamation in Anisotropic Gold Nanorods

Geun Wan Kim, Ji Won Ha^{*}

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Amalgamation is a concentrating process in which metallic gold or silver is mixed with mercury (Hg). Herein, we investigated the plasmon damping of single gold nanorods (AuNRs) caused by mercury amalgamation. First, the time-dependent structural change and the formation of Hg-Au alloy nanorods were studied by scanning electron microscopy (SEM). The aspect ratio of AuNRs decreased due to the mercury amalgamation that resulted in the structural change from a rod to a sphere shape. Second, scattering-based dark-field (DF) microscopy and spectroscopy are powerful tool to characterize optical properties of plasmonic nanoparticles at the single particle level. Thus, in this study DF microscopy and spectroscopy was used to gain new insight into the optical properties and plasmon damping of the Hg-Au alloy nanorods at the single particle level. A strong plasmon damping (or linewidth broadening) in the scattering spectra of single Hg-Au alloy nanorods was observed due to the formation of mercury amalgamation on the AuNR surface. Furthermore, the results indicate that the plasmon damping in single AuNRs can be used as a promising strategy for mercury sensing.

Poster Presentation : **ANAL.P-392**

Analytical Chemistry

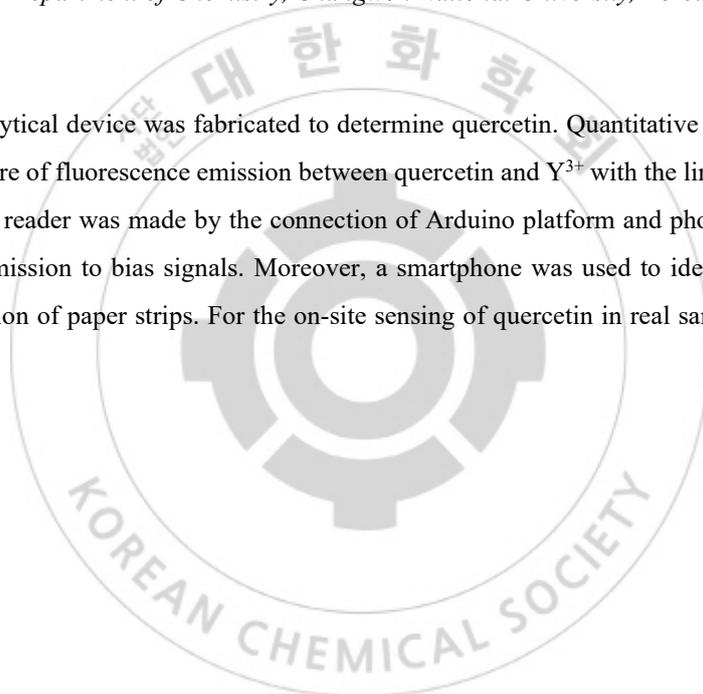
Zoom 10 FRI 15:00~16:00

Quercetin sensor using paper-based analytical devices

Nguyen ngoc Nghia, Bui The Huy, Yong-Il Lee*

Department of Chemistry, Changwon National University, Korea

A paper-based analytical device was fabricated to determine quercetin. Quantitative analysis of quercetin based on the measure of fluorescence emission between quercetin and Y^{3+} with the limit of detection of 27 nM. A home-made reader was made by the connection of Arduino platform and photodiode to transduce the fluorescence emission to bias signals. Moreover, a smartphone was used to identify hue value from fluorescence emission of paper strips. For the on-site sensing of quercetin in real samples, this technique could be used.



Poster Presentation : **ANAL.P-393**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Simultaneous analysis of multiple elements in edible salts by using laser-induced breakdown spectroscopy and laser-patterned silicon wafer substrate

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Salt has various minerals as well as the sodium chloride. Its chemical composition depends on the provenance and the production method, which are the major factors influencing the price in markets. In this study, we used laser-patterned silicon wafer (LPSW) as a sample pretreatment method for simultaneous laser-induced breakdown spectroscopy (LIBS) analysis of multiple elements in edible salts. The newly-devised sample pretreatment method uniformly distributes a small amount of salt solution (15 wt.%) on the silicon wafer surface. A crossed-trench pattern was engraved on the Si wafer in the area of 1 cm × 1 cm using a diode-pumped Q-switched Nd:YLF laser (1053 nm wavelength, 4 ns pulse duration, 1 mJ energy per pulse at 1 kHz, TECH-1053 Express, Laser-export Co. Ltd.). Forty horizontal and forty vertical trenches were engraved with a 250-μm space between two consecutive trenches. Before dropping the salt solution on the LPSW, a hydrophobic scotch tape was attached along the edge of the laser pattern so that the salt solution could be located well inside the patterned area and the homogeneity of dry residues could be improved remarkably. Salt samples were sampled using the LPSWs and then analyzed by LIBS. The intensity of Mg and K obtained through LIBS analysis showed strong correlations with the concentrations determined by inductively-coupled plasma optical emission spectroscopy (ICP-OES) analysis. Also, correlations between K and Mg, and Sr and Ca were investigated for the indirect estimation of K and Sr. This result is expected to be useful not only for rapid and simple salt analysis, but also for the analysis of samples with a limited amount at the level of microliters.

Poster Presentation : **ANAL.P-394**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Analysis of Hydrotreated and Untreated Atmospheric Residue Oil by Atmospheric Pressure Photoionization Cyclic Ion Mobility and ultrahigh-resolution mass spectrometry

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¹Department of Chemistry, Kyungpook National University, Korea

Since crude oil is composed of many compounds within a narrow mass range, ultrahigh resolution mass spectrometry (UHR-MS) is basically an important analytical tool. UHR-MS such as Fourier transfer ion cyclotron resonance mass spectrometer (FT-ICR MS) is an obvious choice to determine the chemical compositions of crude oil, but identifying structural isomers is limited because they cannot be separated. In this study, cyclic ion mobility mass spectrometry (CIM-MS) was combined to enable structural analysis of compounds in crude oil. Atmospheric residue samples before and after hydrotreating process were compared. Samples prepared at 0.5mg/mL in toluene were analyzed in positive atmospheric Pressure Photoionization coupled to CIM and FT-ICR MS. When the drift time obtained from CIM-MS was compared, there was a significant difference between the samples with and without hydrotreating process. The widening of the peak width of the drift time (DT) means that there are many isomers of the compound. The higher the double bond equivalent (DBE), the wider the DT width was observed. As the DBE increased, the structure isomers were also increased. Understanding the structural change occurred by the chemical process is very important because it greatly affects recovery of high-quality petroleum generated during the process. Therefore, the analytical methods shown in this study can provide pivotal platform to study structural changes occurred during hydrotreating of oils.

Poster Presentation : **ANAL.P-395**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Chiral analysis with helical magnetic field induced chiral plasmonic sensor

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Analysis of chiral analytes from small size monomers to large size polymers with chirality has been challenged for effective chiral sensing of drug safety of pharmaceutical. We already have introduced chiral sensing which chiral-active magnetoplasmonic nanoparticles (MNPs) were assembled into helical nanochain structure in helical magnetic field (hB). Ag@Fe₃O₄ core-shell NPs were used for sensing materials that are aligned by a magnetic field. Helically aligned MNP showed remarkable circular dichroism and lead to enhance the CD signals at lower concentration than the technical limit of detection (LOD). This enhancement has successfully occurred in monomers, polymers, and drugs. When left and right polarized light interacted with chiral molecule in hB system, the notable changes of the circularly irradiated light was appeared. Also, different aspects of enhanced signals were observed depending on the type of amino acid. This hB induced chirality enhancer can lead to qualitative and quantitative analysis, which is expected to be applied to the pharmaceutical and biological sensing fields.

Poster Presentation : **ANAL.P-396**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

SERS-based aptasensor for the rapid classification of influenza A & COVID-19 viruses

Hao Chen, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

The ongoing Coronavirus disease 2019 (COVID-19), caused by severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2), has a clear potential for a long-lasting global pandemic, high fatality rates, and incapacitated health systems. More than 100 million cases of Covid-19 have been reported worldwide, including over 2.4 million deaths. Meanwhile, influenza A is also widely spread globally, which has similar symptoms but causes fewer morbidity and mortality. Reverse transcription-polymerase chain reaction (RT-PCR) is the critical diagnostic technique being used. This diagnostic method delivers results with good sensitivity and excellent specificity but is expensive and is slowed by transport to testing laboratories. We aim at designing an aptasensor for inexpensive, simple, rapid diagnostics of SARS-CoV-2 and influenza antigens at the early stage of the disease. Our group has recently developed a SERS-based aptasensor to perform a rapid and sensitive influenza A virus assay. Inspired by our previous work, a dual SERS-based assay platform for the detection of SARS-CoV-2 and influenza A antigens was developed. Herein, a 3D nanopopcorn plasmonic substrate was fabricated using the surface energy difference between a perfluorodecanethiol (PFDT) spacer and the Au layer. Quantitative evaluations of SARS-CoV-2 and influenza virus antigens were performed using a decrease in Raman intensity due to the release of two specific Raman reporter-labeled DNA aptamers from nanopopcorn substrate surfaces via interactions between aptamers and virus proteins. We expect this aptasensor platform to provide new insight into developing a novel platform for rapid classification of COVID-19 and influenza A.

Poster Presentation : **ANAL.P-397**

Analytical Chemistry

Zoom 10 FRI 15:00~16:00

Development of a portable SERS-based lateral flow assay system for on-site diagnosis of SARS-CoV-2

Younju Joung, Jaebum Choo*

Department of Chemistry, Chung-Ang University, Korea

SARS-CoV-2 has spread globally to more than 200 countries, and more than 100 million cases of SARS-CoV-2 have been reported worldwide. A rapid and accurate test for SARS-CoV-2 is urgently needed to control the spread of the viruses. Reverse transcription-polymerase chain reaction (RT-PCR) has been considered a gold standard for detecting SARS-CoV-2 target genes. In RT-PCR, however, the total diagnostic time, including sample preparation, gene amplification, and detection, takes approximately 3-4 hours. Thus, it is necessary to shorten the diagnostic time for rapid on-site diagnosis. Various rapid kits for immunodiagnosis using antigen-antibody reactions were also developed to shorten the diagnosis time. However, they have not been adopted as the standard diagnostic method due to their low accuracy. In particular, the “false-negative” problem of commercialized immunodiagnostic kits is recognized as a severe problem that can aggravate the spread of the SARS-CoV-2. To resolve the issues, we have developed a SERS-based lateral flow assay (LFA) sensor with a portable Raman reader for rapid and sensitive immune analysis of SARS-CoV-2. We believe that the portable SERS-based LFA sensor enables on-site diagnostics of SARS-CoV-2. The quantitative evaluation of SARS-CoV-2 in a transport medium solution containing nasopharyngeal swabs is possible. Our SERS-based LFA sensor shows a strong potential to resolve the problems in terms of low sensitivity and limit in quantitative analysis inherent in conventional antigen tests to detect SARS-CoV-2.

Poster Presentation : **ANAL.P-398**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Quantitative Analysis of Al and V Concentrations in Ti-6Al-4V Alloy Using CF-LIBS

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Ti-6Al-4V alloy is also known as Ti64, TC4, or ASTM Grade 5, is an alpha-beta titanium (Ti) alloy. It has high strength, low density, high heat resistance, excellent weld-ability, high fracture toughness, excellent corrosion resistance and also provides better biocompatibility. It is generally recognized as the most popular Ti alloy and occupies almost 50% of the market share of Ti products used in the world today. In present work, we have analysed the concentrations of Al and V in the Ti64 alloy (NIST SRM 654b) using calibration-free laser-induced breakdown spectroscopy (CF-LIBS). It is an alternative approach that requires no calibration standards for quantitative analysis like conventionally LIBS. However, certain conditions related to the temperature and electron density of the plasma based on the assumptions of local thermal equilibrium, stoichiometric ablation, and optically thin plasma are required to be fulfilled strictly. The LIBS spectra of the Ti64 alloy were recorded in the wavelength range between 388 and 428 nm at altered gate delays i.e. 0.2, 0.7, 1.2, 1.5, 1.7, 2.2, 2.7 and 3.2 μ s. At each gate delay, thermodynamic parameters (plasma temperature and electron density) and concentration of Al and V were calculated. The results estimated at 1.7 μ s gate delay were best amongst all gate delays and provides better accuracy when compared with the certified values, i.e. 6.34 wt. % for Al and 4.31 wt. % for V in the Ti64 alloy. The concentrations of Al and V were estimated at 1.7 μ s found to be 5.79 ± 0.92 wt. % and 4.07 ± 1.18 wt. %, respectively. Our results suggest that tuning gate delay would provide better quantification of Al and V concentrations in Ti64 alloy using CF-LIBS.

Poster Presentation : **ANAL.P-399**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Development of tissue-specific classification by hyperspectral autofluorescence images

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Hyperspectral imaging-based tools have been developed as a strong candidate which can replace time-consuming histopathological analysis. Hyperspectral image contains the spectral profile on each point of image that constitute hyperspectral cube which provide chemical/biological information with high spatial resolution. Hyper Spectral imaging based on tissue autofluorescence by endogenous fluorophores (Collagen, Elastin, NADH, FAD...) has been applied to analyze biological nature or metabolic change. Depending on the composition and level of metabolism, spectral changes can be caused, which can act as biomarkers to reflect cancer tissue characteristics. To this purpose, we obtained a hyperspectral autofluorescence image of the tissue section. We preprocessed hyperspectral image by spectral calibration and baseline correction and the resulting image was labeled with the characteristic compartmentalization of tissue by pathological analysis to learn the supporting vector machine (SVM) model. The SVM model include the process of selecting the features with the most consistency with pathological analysis among the various features obtained from fluorescence data. Consequently, we could provide compartment maps which showed similar classifying results to pathological analysis.

Poster Presentation : **ANAL.P-400**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

LC/MS-based polar metabolites analysis after axon regeneration in peripheral nerve-injured mouse

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Peripheral nerve damage causes severe sensory and motor dysfunction. However, after peripheral nerve injury, axon regenerate and function is restored. Therefore, the process of axon regeneration after nerve injury is important and metabolic studies are needed. We observed changes in polar metabolites of axon regeneration in nerve-injured mouse. In this study, we performed the non-targeted polar metabolomic profiling of dorsal root ganglion (DRG) tissue from mouse using ultra performance liquid chromatography/quadrupole time of flight mass spectrometry (UPLC/Q TOF MS). 10 control mice and 10 nerve-injured mice with regenerated axons after sciatic nerve crushing were analyzed. Multivariate analysis showed discriminated metabolic pattern between control group and nerve injury group. Non-parametric t-test was used to find significantly different metabolites between control group and nerve-injured group. As a result, glutathione, histamine, N-acetylaspartate, creatinine, N-acetylaspartylglutamic acid, D-fructose 6-phosphate significantly decreased, whereas glutathione oxidized, leucine, glutamate, histidine, phenylalanine, glutamine, uridine, UDP-N-acetylglucosamine significantly increased after nerve-injured mice. Pathway analysis revealed that significant metabolic pathway were glutathione metabolism, alanine, aspartate and glutamate metabolism and histidine metabolism in nerve-injury mice. These results showed that polar metabolites were changed after axon regeneration in nerve-injured mouse compared to control. This study demonstrates that the LC-MS based non-targeted polar profiling can be a used to understand the mechanism of axon regeneration in peripheral nerve-injured mouse.

Poster Presentation : **ANAL.P-401**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Enhanced Signal Boosts of Silicon Nanoparticles via Selective ^{29}Si Isotope Enrichments for DNP-MRI Applications

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Nuclear Magnetic Resonance (NMR) spectroscopy is one of the principal analytical tools for biological applications since the method provides structural information and molecular interactions. However, due to severe sensitivity issues originated from both low magnetic moments and low natural abundance of NMR active nuclei, except hydrogen atom, there are many restrictions conducting NMR experiments in general conditions. Dynamic Nuclear polarization (DNP) is one of the strong tools to enhance the sensitivity of the NMR signal by transferring the high polarization level of electron spins to low polarization level of nuclear spins using microwave irradiation. Another powerful tool is isotope enrichment, which is the most direct way to increase the signal by increasing the amount of NMR active nuclei. In this research, we experimented by applying these two methods to silicon nanoparticles. A DNP experiment was proceeded by synthesizing particles having 10% and 15% ^{29}Si nanoparticles based on the 4.67% silicon nanoparticle, which is the natural abundance of silicon. To determine the effect of enrichment, the signal of enriched silicon nanoparticles is measured in DNP-NMR, and the build-up constant and T1 relaxation time are calculated through build-up and decay test. After that, the MRI phantom image is measured to make sure whether the signal amplification by DNP is detected within the MRI. Finally, the possibility as an imaging agent is confirmed through an in vivo experiment using a mouse. This research is expected to contribute examining effect of enriched-silicon as potential molecular imaging probes.

Poster Presentation : **ANAL.P-402**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

¹H NMR-based metabolomic profiling to identify the treatment effect of acupuncture in patients with functional dyspepsia

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Functional dyspepsia (FD) is a common functional gastrointestinal disorder in clinical gastroenterology with multiple pathogenic mechanisms. Many possible factors including abnormal neurohormonal function, autonomic dysfunction, visceral hypersensitivity or mechanical distention, psychosocial comorbidity and stress are to be considered in the pathogenesis of FD. Acupuncture, an important therapeutic method based on meridian theory in traditional Chinese medicine, has been shown to be effective for the manipulation of abnormal physiological conditions in the human body and for the treatment of various functional diseases such as FD. However, there are few metabolic studies relevant to the treatment effect of acupuncture in FD patients. In this study, we analysed urinary and serum metabolites to investigate the treatment effects of acupuncture in FD patients. We performed metabolic profiling using nuclear magnetic resonance (NMR) spectroscopy to investigate metabolites in urine and serum samples from patients with FD. Several metabolites were significantly changed in urine and serum sample of FD patients who received acupuncture treatment, and it was confirmed that specific metabolite could be a marker proving effective acupuncture treatment in FD patients. This study demonstrates that the urinary and serum metabolites of FD patients were changed after acupuncture treatment, and metabolomics approach can be used to investigate the treatment effects of acupuncture in FD patients.

Poster Presentation : **ANAL.P-403**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Spiral Scanning System for Ultrafast Quantitative analysis of Pesticide with flexible SERS substrate

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Surface enhanced Raman spectroscopy (SERS) has proven to be a sensitive tool for probing harmful chemical residues in various substances such as food, water, and soil. Although SERS signal lower the limit of detection (LOD), but non-uniformity SERS substrates have different SERS intensity depending on the analysis location, so the homogeneity on the SERS substrate must be considered to ensure the reliability in quantitative analysis. Also, in the process of preparing analytes on the SERS substrate such as drop casting or dipping, non-uniform adsorption inevitably occurs because of surface structure. The limitations of quantitative analysis due to this heterogeneity can be overcome by repeated measurements of numerous spots, although it requires extensive measurement time. In this study, we developed a spiral scanning system that provide rapid and quantitative SERS measurements using fast spinning rotor flexible SERS substrates. We evaluated the reproducibility of SERS signal both for multi-spot Raman sampling and for spiral scanning systems. We note that the magnitude of error bar is significantly smaller for spiral scanning measurements than conventional multi-spot sampling.

Poster Presentation : **ANAL.P-404**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

The Structural Studies of Biomimetic Peptides P99 Derived from Apo B-100 by NMR

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Apolipoprotein B-100 (apo B-100), the main protein component that makes up LDL (Low density lipoprotein), consists of 4,536 amino acids and serves to combine with the LDL receptor. The oxidized LDL peptides by malondialdehyde (MDA) or acetylation in vivo were act as immunoglobulin (Ig) antigens and peptide groups were classified into 7 peptide groups with subsequent 20 amino acids (P1-P302). The biomimetic peptide P99 (KGTYG LSCQR DPNTG RLNGE) out of B-group peptides carrying the highest value of IgM antigens were selected for structural studies that may provide antigen specificity. Circular Dichroism (CD) spectra were measured for peptide secondary structure in the range of 190-260 nm. Experimental results show that P99 has pseudo α -helice and random coil structure. Homonuclear (COSY, TOCSY, NOESY) 2D-NMR experiments were carried out for NMR signal assignments and structure determination for P99. On the basis of these completely assigned NMR spectra and proton distance information distance geometry (DG) and molecular dynamic (MD) were carried out to determine the structures of P99. The proposed structure was selected by comparisons between experimental NOE spectra and back-calculated 2D NOE results from determined structure showing acceptable agreement. The total Root-Mean-Square- Deviation (RMSD) value of P99 obtained upon superposition of all atoms were in the set range. The solution state P99 has mixed structure of pseudo α -helix and β -turn(Gln[9] to Thr[13]). These NMR results are well consistent with secondary structure from experimental results of circular dichroism. Structural studies based on NMR may contribute to the prevent oxidation studies of atherosclerosis and observed conformational characteristics of apo B-100 in LDL using monoclonal antibodies.

Poster Presentation : **ANAL.P-405**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

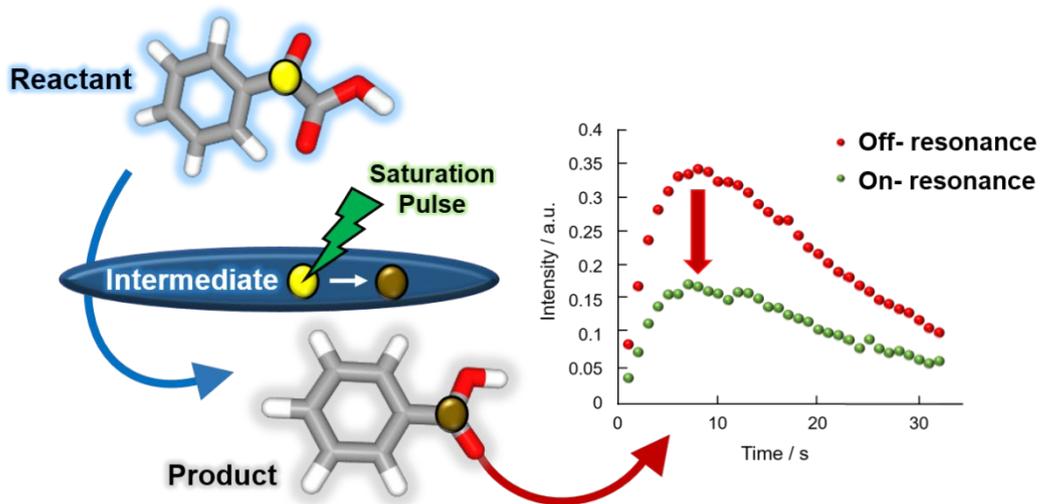
Invisible reaction intermediate studies in decarboxylation reaction of phenylglyoxylic acid and hydrogen peroxide by blind saturation using D-DNP

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D-DNP (Dissolution-dynamic nuclear polarization) technique can enhance NMR signal by several orders of magnitude, allowing NMR spectroscopy to investigate reaction mechanisms and kinetics in real time. However, in preliminary mechanism studies using D-DNP, reaction intermediates with a sufficiently high stability and population during the NMR measurement time were observable. Here, we conducted blind saturation experiments using D-DNP to demonstrate whether invisible intermediates of unlabeled compounds can be identified in decarboxylation reaction between α -keto acid and hydrogen peroxide. First of all, a prior study using 1,2-¹³C pyruvate was carried out and it was observed that the product signal decrease as applying a selective saturation pulse to the intermediate of pyruvate. Subsequently, phenylglyoxylic acid (PHGA) was used to conduct a "wide" selective saturation experiment, showing that the reaction intermediate of PHGA is present in a region of 99 to 105 ppm similar to pyruvate. To acquire more accurate chemical shift information of PHGA intermediate, a "narrow" selective saturation experiment was proceed and the pulse was applied at an excitation range of 1 ppm while changing the frequency center within 99 to 105 ppm. As a result, it was possible to determine the chemical shift information about intermediate of PHGA, observing that the intensity of product was significantly reduced when selective saturation is applied at 103 ppm. In conclusion, we successfully obtained the chemical shift of reaction intermediate not visible in NMR spectrum through blind selective saturation method which is expected to be effectively used to identify important and complex chemical and biological pathways.



Poster Presentation : **ANAL.P-406**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

The Efficacy of Antibacterial Feed to evaluate Bacterial Diseases Resistance in *Paralichthys Olivaceus*

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In the previous study, the efficacy of antibacterial feed was analyzed by detecting the protein expression of *Paralichthys olivaceus* (*P. olivaceus*) before and after feeding the antibacterial feed. After feeding antibacterial feed for 4 weeks, this study further intends to analyze the disease resistance by detecting the protein expression of *P. olivaceus* which was artificially infected with *Streptococcus iniae* (*S. iniae*). Among the bacterial diseases, *S. iniae* is known to infect many fish species and is therefore, an important causative agent of streptococcosis in *P. olivaceus* culture. Proteins were extracted with RIPA buffer from homogenized head kidney tissues of *P. olivaceus*. Each supernatant fluid was pooled into three groups according to time period after artificial infection. Pooled samples from *P. olivaceus* were trypsin digested and desalted. After that, the proteins in three groups were analyzed with nLC-MS/MS and protein database searches. The disease resistance as efficacy of the antibacterial feed was evaluated with differentially expressed protein (DEP) and gene ontology (GO) enrichment analysis.

Poster Presentation : **ANAL.P-407**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Bio 3D printing ink and scaffold containing bone regenerate mineral nanoparticles

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Whitlockite is a calcium phosphate-based ceramic. It contains Mg²⁺ ions, which plays an important role in bone metabolism like bone growth and osteoporosis. As the second most abundant mineral in living bone, Whitlockite occupies 25–35 wt % of the inorganic portion of human bone. We are going to make bone-like bio 3D ink and scaffold using whitlockite and hydroxyapatite and analyze them. That's because 3D printing technology is necessary to output a customized implant to be applied during surgery in-situ. The 3D printing ink and scaffold is composed of whitlockite synthesized by a large-scale precipitation synthesis method and a small amount of polyvinyl alcohol (PVA) was made using an inkjet 3D printer. The bio-ink and scaffold were shown by scanning electron microscopy (SEM), porosity, Thermogravimetric analysis (TGA), and compressive strength testing. These results suggest that whitlockite has excellent potential for application in bone tissue engineering.

Poster Presentation : **ANAL.P-408**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Enzymatic Mechanism Studies of Biodegradable Natural Polymer based Microcapsule using ^1H Nuclear Magnetic Resonance Spectroscopy

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Developing biocompatible microcapsules instead of microplastics is receiving much attention for environmental protection, and the biodegradation of microcapsule can be analyzed by FTIR, HPLC, TGA or using the standard OECD test. However, NMR can be used as potential analysis method applied in the study of polymer-based microcapsules with providing detailed structure and degradation mechanism. Here, we attempt synthesizes biodegradable microcapsule and proposes enzymatic degradation mechanism of microcapsule utilizing ^1H -NMR. Synthesis of microcapsule were characterized by IR, Microscopy and SEM, indicating the interaction between alginate, gelatin, and linker. Also, it showed spherical and uniform shape, with particle size from 20 μm to 30 μm . The cleavage of alginate polymer was observed due to the enzyme through NMR analysis over time, and real-time glucose production was monitored through the DNS method. Also, in control experiment, the microcapsules showed relatively high stability in simple PBS buffer, so that enzyme-induced biodegradation could be demonstrated. Morphology changes of sample due to the enzyme were examined by microscopy as well as SEM. According to SEM results, Microcapsule particles started to burst after 1 week and almost disappeared after 2 weeks incubation. NMR results showed the kinetic and mechanism information of microcapsule followed Gouy model that was obtained by $\Delta 4\text{G}$ (5.89ppm) and $\Delta 4\text{M}$ (5.76ppm) with high corresponding values are 0.997 and 0.956, respectively. Also, the kinetic study of microcapsule was obtained by UV showed similar kinetic modeling. In future study, we will develop a new multifunctional polymer that can be used in biodegradable microcapsules, as well as the mechanism study currently being conducted.

Poster Presentation : **ANAL.P-409**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Photocatalytic Reactivities in Closely Packed Cavities by Au Nanocrystals

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Plasmonic metal nanoparticles have been receiving increasing attention as visible-light-driven photocatalysts due to their unique optical property by localized surface plasmon resonance (LSPR). However, metal nanoparticle based-photocatalysts have essential limitations that the rate of recombination of excited electrons and holes is too fast so that these charge carriers cannot sufficiently participate in chemical reactions. As a consequence, the reaction rate in plasmonic photocatalyst is governed by the diffusion rate of a chemical substance to near the photocatalysts, resulting in showing a slower reaction rate. Thus, a key strategy to improve the rate of reaction in plasmonic photocatalysts is that either diffusion length of a chemical substance as an electron acceptor or migration length of the excited electron, which can participate in a chemical reaction, have to be shortened. In this study, we designed the confined cavities, where the chemical substance can be captured, to reduce the distance between photocatalysts and the reaction species. And, we not only examined the electron transfer kinetics in plasmonic photocatalyst between the free-standing colloidal system and the aggregation-induced system but also compared the reaction kinetics between gold nanoparticles and gold nanoclusters.

Poster Presentation : **ANAL.P-410**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Synthesis of Au NPs@Poly(acrylic acid) Nanocomposite via Interaction of Au Nanoparticles and Visible Light

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Researches of polymeric nanocomposites are notable in chemistry, biochemistry, biology, and material science because they can be applied in a variety range of applications in industry as well as our daily life. Especially, the polymeric nanocomposite is able to a potential material that has a great advantage to use for liquid crystal, polarized film, thermal therapy, bio-imaging, and drug-delivery. Plasmonic Au nanoparticles have been receiving much attention in catalysis and bio-applications due to a unique optical property that resulting from the interaction with electromagnetic radiation. When the plasmonic nanoparticles like Au nanoparticles absorb light, the energetic charge carrier, called hot electrons, and the thermal energy are generated in the vicinity of nanoparticles. Both energies such as the hot electrons or thermal energy have large enough energy to initiate the polymerization process on the surface of nanoparticles. Many kinds of photo-polymerization researches have been published, however, the main factor of photo-polymerization has still remained unclear. In this study, we investigated the main influence of photo-induced polymerization by controlling incident wavelength, polymerization time, reaction conditions, and etc. We monitored the absorption spectra of synthesized Au NPs@PAA with a UV-Vis spectrophotometer to observe the change in dielectric constant near Au nanoparticles and the morphological change was confirmed using TEM. Also, we investigated the chemical structure of the products using FT-IR and other analytical tools.

Poster Presentation : ANAL.P-411

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Simulation of Modified the Morphology of Fe Complex Nanorods Photoanode with Diverse Aspect Ratio for Enhancing the Efficient Oxygen Evolution Reaction

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The hydrogen production thorough the photoelectrochemical (PEC) water splitting ($2\text{H}_2\text{O} \rightarrow 2\text{H}_2 + \text{O}_2$) system is promising system to store solar energy in a clean, low-cost, efficient, and large-scale. Water-splitting technologies depend on a series of electrochemical reactions such as oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) on the electrode surface. The quantity of evolution is able to check the chemical activity of the electrode. However, the reactions have many obstacles to produce oxygen and hydrogen. One of the main problems for the overall efficiency of water splitting is the sluggish kinetics of OER, which involves multiple steps of proton-coupled electron transfer. To defeat the kinetic barrier at a relatively high chemical activity, cost-effective and highly efficient catalysts are required. Herein, the alignments of the Fe complex nanorods along the different magnetic fields are introduced. This nanorods supported on Fluorine-doped tin oxide (FTO) glass facilitates the diffusion of gaseous products (hydrogen and oxygen). Therefore, tuning the electronic structure toward having a chemically active surface area on electrode enhances the chemical activity and outstanding stability for OER in alkaline electrolyte.

Poster Presentation : **ANAL.P-412**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Colorimetric Detection of Mycobacterium tuberculosis in Clinical Samples using Au@Pd Nanoparticle-Based Magnetic Enzyme-Linked Immunosorbent Assay

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The development of sensitivity and point-of-care diagnostic tools for serum profile of numerous Mycobacterium tuberculosis (MTB) corrects existing tuberculosis diagnostic deficiencies. Herein, an ultrasensitive antigen-based tuberculosis detection technique and a bacterial growth monitoring strategy were designed using two nanozyme probe-based colorimetric enzyme-linked immunosorbent assay (ELISA). An anticulture filtrate protein-10 (CFP-10) factionalized magnetic nanobead (MNB) probe segregated the CFP-10 antigens from clinical samples, whereas the Au core and Pd shell (Au@Pd) nanozyme detection probe catalytically oxidized the commercially available chromogenic substrate 3,3',5,5'-tetramethylbenzidine (TMB) to yield a concentrationdependent color tonality as a signal indicator. This NZ-based colorimetric ELISA presents a robust and sensitive analytical technique for antigen-based clinical diagnosis, with potential applications in the clinical field, as well as for other epidemic diseases.

Poster Presentation : **ANAL.P-413**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Self-assembly of magnetoplasmonic nanoparticles by helical magnetic field and its applications

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Circular dichroism (CD) could be measured the absorbance difference of left and right circularly polarized light (LCP and RCP). In order to arrange the anisotropic and asymmetric of plasmonic nanomaterials, most researchers used DNA template to attach nanoparticles. However, it was difficult to control the optical properties due to the structural rigidity of the template. We developed a device that combined with CD and magnetoplasmonic nanoparticles (MNP), which has magnetic and plasmonic properties under the helical magnetic field. Therefore, the chiroptical property of MNP chain can be controlled by adjusting distance of two magnets. This research can be applied at biosensing and imaging.

Poster Presentation : **ANAL.P-414**

Analytical Chemistry

Zoom 10 FRI 16:00~17:00

Colorimetric Strain Sensor made by Magneto plasmonic photonic crystal array on a flexible substrate

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Recently, many people have challenged wearable devices. Wearable devices need to be able to constantly exchange information with users through sensors. Sensors used to detect various conditions output information in many cases as electrical signals. Signals transmitted as electrical signals have many advantages, but the need for low power, flexible sensors for long time use is increasing. The plasmonic 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. In the papers describing the color change using nanoparticles, most use plasmonic noble metal as a particle. Plasmonic noble metal particles form a plasmon coupling forming a chain structure and has plasmon resonance on the surface. The reflectance of the surface is changed by physical force, and this characteristic is used in color sensors. For example, Au noble metal colloidal nanoparticles can be seen using plasmon resonance characteristics to show a color change. Ag@MNPs a film sensor using nanoparticles can visually represent a physical change and apply it to various movements. Besides, the advantage of being able to change the color of the sensor depending on the size of the nanoparticles will be used in a wide range during the actual application. In this paper, only physical reactions will show that the color changes without current and explain the principle. This will be able to achieve the purpose as a sensor by showing a definite change that differs from the saturation or brightness. To solve this 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-415

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Facile Synthetic Methods of Magnetic Carbon Nanoparticles with Different Morphological Features and its Application on Adsorption / Adsorption Mechanism of Organic Substances

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Magnetic carbon nanomaterials were used extensively as an adsorbent in the last two decades due to high surface area and easy recovery. Herein, we present a comparison of three magnetic carbon nanosphere (MCNs), which are synthesized from polydopamine (PDA) and iron or iron oxide nanoparticles (Fe₃O₄ NPs) for adsorption methylene blue (MB). Three MCNs are prepared with similar size (~200 nm) and spherical morphology, including multi-core, core-shell, and linker structures. Many previous studies utilized the multi-core and core-shell structure in their reports, the linker is new material in our research. It is designed by carboxylic acid-functionalized activated carbon nanospheres (ACNs-COOH) connected with amine-terminated iron oxides NPs (Fe₃O₄-NH₂) through the carbodiimide crosslinking reaction. Therefore, linker material is shown the highest specific surface area and strong magnetism. Because of this reason, the linker sample exhibits the highest maximum adsorption capacity based on the Langmuir isotherm model at pH=10 for removal MB; and it can separate easily by an external magnetic field. Moreover, we proposed the adsorption mechanism of three MCNs through electrostatic interaction, π - π interaction, and intraparticle diffusion kinetic model.

Poster Presentation : **ANAL.P-416**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Four-dimensional light sheet-based non-fluorescent super-resolution microscopy for minimizing optical illusion

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Light-sheet super-resolution microscopy (LSRM) is an essential methodology to visualize the sample in depth which is the competent detection technique for biological molecules compared to other tools while having a limitation by uneven light path as a result of solid-angle illumination. Optical illusion is an observation barrier of the single-molecule in diffraction limitation based on illumination limitation in LSM. In this work, we present the four-dimensional light sheet-based non-fluorescent super-resolution microscopy (4D LNSRM) to minimize the optical illusion. 4D LNSRM system was integrated with total internal reflection and differential interference contrast (DIC) microscopy. A rotatable cuboid prism in the 4D LNSRM system simply overcame the optical illusion by rotating the specimen on the prism to change the direction of light that comes from illumination lens with high-resolution imaging. LNSRM 3D reconstructed images of nanoparticles mixture (20 nm AgNP, 100 nm AuNP, and 250 nm AuNP) were acquired in multi-illumination angles of 0°, 90°, 180°, and 270°, which complicated the 4D imaging (3D super-resolution imaging + multi-angle illumination).

Poster Presentation : ANAL.P-417

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Comparison of Competitive and Sandwich Immunoassays on Gold Nanoarray Chip by Total-Internal Reflection Fluorescence Microscopy

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Immunoassays include a competitive assay which causes the antigen to react competitively to the antibody and a sandwich assay which uses a pair of antibodies for the target. The competitive assay is used to accurately determine the antigen concentration in a sample, simplifying the diagnostic procedure using a single antibody. In addition, the sandwich assay is used for quantitative analysis due to its high sensitivity, specificity, and precision. Herein, we investigated the difference of the sandwich and competitive reactions on gold nanopatterned array chips by total internal reflection fluorescence microscopy (TIRFM). Fluorescence signal of small size analytes were detected by TIRFM through competitive reaction on gold nanoarray chips. As a result, a wide dynamic range was obtained with high sensitivity and selectivity. In addition, the competitive reaction showed shorter analysis time than that of the sandwich reaction, but the reaction conditions need longer time to obtain the appropriate sensitivity and range. In comparison, the sandwich reactions could be detected with higher sensitivity and accuracy using many analytes with multiple binding sites.

Poster Presentation : **ANAL.P-418**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Real-time Single Particle Tracking of Anisotropic Nanoparticles by Light Sheet Super-Resolution Microscopy

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A light sheet super-resolution microscopy (LSRM) for real-time tracking and translational and rotational movements of individual anisotropic nanoparticle in solution was developed. This approach combined astigmatism method and polarized light sheet excitation. Native gold nanorod (AuNR; 5 nm diameter × 15 nm length) were used as imaging nanoprobe to detect its motional behaviors in solution. The translational and rotational dynamic differences of native AuNR and surface modified-AuNR in solution were monitored in real time. Owing to frictional force between AuNR and solution, surface modified-AuNR moved more slowly and rotated more difficultly. The LSRM was shown to be reliable and useful in the field of non-fluorescence super-resolution imaging and real-time single particle tracking in solution.

Poster Presentation : ANAL.P-419

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

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

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

Poster Presentation : **ANAL.P-420**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Enhanced electrochemical properties of iodine doped LiFeBO_3 as a cathode for lithium-ion battery

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As a cathode material for high-capacity lithium-ion batteries, LiFeBO_3 (LFB) has a higher theoretical capacity of 220 mAh/g than that (170 mAh/g) of LiFePO_4 and is eco-friendly and inexpensive. Due to the disadvantage of poor electrical conductivity, however, various studies have been conducted to improve this characteristic. Herein, we have studied to improve the electrical conductivity by doping iodine having high electronegativity in oxygen sites of LiFeBO_3 . Iodine doped $\text{LiFeBO}_{3-x}\text{I}_{2x}$ has been synthesized by solid-state reaction using planetary ball mill. Solid-state NMR and XRD have been measured to characterize the microstructure and crystal structure of prepared material. Via XRD pattern, it is confirmed that monoclinic single-phase is changed to vonsenite-like phase by iodine doping in LFB. This phase transition to vonsenite can be expected to increase the theoretical capacity. To observe the effect of iodine doping on the electrochemical properties, the electrochemical performances of the synthesized material have been studied by Galvano static charge/discharge test.

Poster Presentation : ANAL.P-421

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Metabolite profiling of *Nymphaea nouchali* (Burm.f) stem using high resolution mass spectrometry and attenuation of t-BHP-induced oxidative stress in RAW264.7 cells via modulation of MAPK/Nrf2/HO-1/ROS signaling cascade

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Identification of the secondary plant metabolites of the methanol extract of *Nymphaea nouchali* stem (NNSE) were carried out using high-resolution mass spectrometry (HRMS). The antioxidant effects of the NNSE as well as underlying mechanisms were investigated in t-BHP stimulated oxidative stress in RAW264.7 cells. Tandem mass spectrometry with negative mode electrospray ionization (ESI) tentatively revealed the presence of 54 secondary metabolites in NNSE, among them phenolic acid and flavonoids were predominant. Phenolic acid, sialic acid and terpenoid as brevifolincarboxylic acid, 2-deoxy-2,3-dehydro-N-acetylneuraminic acid, and α - β -Onoceradienedione were found in NNSE for the first time. The NNSE had strong free radical scavenging capabilities, which also able to reduce t-BHP induced cellular ROS generation in RAW264.7 cells. The NNSE extract was found to prevent oxidative stress by boosting the levels of HO-1 through upregulation of Nrf2 via the regulation of MAPKs such as p38 and JNK phosphorylation in RAW 264.7 cells. These results scientifically advocate the potentiality of NNSE for defending oxidative stress stimulated diseases. Keywords: antioxidant; *Nymphaea nouchali*, heme oxygenase 1 (HO-1); nuclear factor erythroid 2-related factor 2 (Nrf2), RAW264.7 cells

Poster Presentation : **ANAL.P-422**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Synthesis and characterization of LiMBO_3 as a cathode material for lithium secondary batteries

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Researches on polyanionic structured lithium metal borate material, LiMBO_3 ($M = \text{Mn, Fe or Co}$), as a cathode material for lithium secondary batteries have been actively conducted due to its light weight, structural stability, and high theoretical capacity (220 mAh g⁻¹). Herein, $\text{LiMn}_{1-x}\text{Co}_x\text{BO}_3$ and $\text{LiFe}_{1-x}\text{Co}_x\text{BO}_3$ ($x = 0, 0.25, 0.5, 0.75, \text{ and } 1.0$) have been synthesized by sol-gel method. To characterize the crystal structure and microstructure, X-ray diffraction (XRD) and solid phase ⁷Li MAS NMR spectroscopy have been measured. In addition, via Galvano static charge/discharge test, oxidation/reduction potentials and operating voltage have been studied. Quantitative analysis for chemical composition of materials has been also performed with laser induced breakdown spectroscopy (LIBS).

Poster Presentation : **ANAL.P-423**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

A study on the separation of arsenic species by capillary column

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IARC under the WHO classifies arsenic as a carcinogen in Group I. We are exposed to arsenic mainly from the drinking water and food, and the chronic exposure can cause the problems such as peripheral nerve disease. The chemical species of arsenic has been very critical because their toxicity depend on the chemical forms. Thus, the accurate determination of total arsenic and arsenic species has been an important issue. There are already various methods of separation of arsenic species using a general column such as cationic and anionic separator column. The general columns typically use 100 ~ 1000 μL volume sample loops. The necessary amount of sample should be three times larger than the sample loop volume for analytical measurement, and the system could not often apply on the limited samples such as clinical and biological samples. Therefore, we studied a method of separating arsenic species in a limited sample using a capillary column with a small sample loop of 5 μL . 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 linear calibration curves from 1 $\mu\text{g}/\text{kg}$ to 50 $\mu\text{g}/\text{kg}$ were obtained for inorganic arsenic. The recovery efficiency of 20 $\mu\text{g}/\text{kg}$ As^{5+} was 97.54 %.

Poster Presentation : **ANAL.P-424**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Simple Infrared spectroscopic identification of faulty pre-coated metal products

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PCM, a pre-coated metal panel used in the manufacture of various home appliances, can be easily processed into the intended form of the target product, making it easier to mass-produce and further improving the appearance of the product. So, the quality of PCM paint during the production process is more important to ensure the high value of PCM-based products. For that reason, defects in PCM substrates are one of the most challenging tasks, and simple analysis methods are required to quickly identify defects in products. In this study, infrared (IR) spectroscopy has been used to identify faulty 1) grey-silver PCMs contained with and without a phosphate epoxy (2.0%), 2) normal and violet colorant-contaminated (0.2%) black PCMs, and 3) normal, violet colorant-contaminated (0.5%), and yellow colorant-contaminated (0.1%) white PCMs samples. A strategy for improving the accuracy of the identification analysis, a temperature-perturbed infrared measurement was incorporated with 2T2D correlation analysis. When 2T2D correlation analysis was conducted using spectra with temperature changes, the identification of the three sample groups were significantly improved over the principal component analysis. According to the 2T2D correlation analysis, the effectiveness of capturing different spectral variation between the normal paint PCM and the defective paint PCM by temperature contributed to the improvement in identification.

Poster Presentation : **ANAL.P-425**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Lipidomic profiling on the effects of particulate matter exposure in mice using LC-MS approach

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Particulate matter (PM) is major environmental risk factors in worldwide, and related to human such as respiratory organ, cardiovascular, and nervous system. Recently, many researches have been reported effect by exposure to PM in biological system, whereas the molecular mechanism is not clear. We observed the metabolic changes in response to PM with a diameter 2.5-10um (PM10) exposure in mouse model. In this study, C57BI/6J mice (male) were exposed to PM10 or clean air for 3weeks in chambers. We performed global lipid profiling of hippocampus from mice to estimate metabolic alteration using ultra performance liquid chromatography/quadrupole time of flight mass spectroscopy (UPLC/Q TOF MS). We identified 300 lipids in hippocampus. Partial least squares - discriminant analysis (PLS-DA) score plots showed a separation between the PM10 group and control group. We found changes in lipid such as free fatty acid, ceramide, diacylglycerol and phospholipid species in PM10 exposed to mice compared to control. Most of phospholipid species were increased in PM10 exposed mice compared to control, whereas free fatty acid, ceramide and diacylglycerol species were decreased in PM10 exposed group. This study demonstrates that the LC-MS based-lipid profiling can be a used to understand the metabolism of PM10 exposed group on biological system.

Poster Presentation : **ANAL.P-426**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Development of a low-cost Do-It-Yourself (DIY) air sampler for TD-GC/MS analysis

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A Do-It-Yourself (DIY) air sampler was developed to sample the sorbent tubes used in thermal desorption-gas chromatography mass spectrometry (TD-GC/MS). In GC/MS analysis, TD is often used as a pre-concentration method prior to injection of the low concentration gas sample. In order to use TD, gas sample should be collected into a tube filled with adsorption material using an equipment called an air sampler. Since the commercially available air samplers are expensive at a price between \$1,000 and \$2,000, a DIY air sampler was developed to replace it. This air sampler can be made under \$90 and all materials required for production are released as open-source. Furthermore, the performance of the air sampler is validated by TD-GC/MS analysis using the BTEX (benzene, toluene, ethylbenzene, and o-xylene) samples.

Poster Presentation : **ANAL.P-427**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Site-specific TEMPO mediated FRIPS for a model protein using genetically incorporated unnatural amino acid: Structure dependent radical dissociation of protein

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The radical driven dissociation using TEMPO mediated FRIPS is a powerful approach for peptide sequencing under collisional activation. It provides efficient analysis of peptides having disulfide bonds or post-translation modifications like other radical based techniques because fragmentation mechanism follows nonergodic process. However, the previous method has a limitation in introducing the TEMPO based reagent at a desired site because the conjugation unit, -NHS functional group, can only conjugates with primary amines, generally only with N-terminal amine after blocking lysine residues. In this study, we suggested the site-specific TEMPO mediated FRIPS for protein structure analysis using genetically incorporated unnatural amino acid, where one of the residues in model protein (affibody) was modified to acetylphenylalanine, followed by the conjugation of modified TEMPO based reagent. We chose multiple modification/conjugation sites considering the three-dimensional structure, and the tandem mass spectrometry experiments were conducted. The results showed that the sites of radical driven fragmentation were closely related to the modification/conjugation sites. We are conducting additional experiments to obtain clear relationship between the radical position and protein structure by differing the modification/conjugation sites. We anticipate that this approach could provide a new way to the elucidation of protein structure.

Poster Presentation : **ANAL.P-428**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Development of the screening software for the identification of unknown narcotic drugs through the machine learning models and hybrid similarity searches

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A software for screening unknown narcotic drugs using the machine learning based models and search algorithms was developed. The screening of unknown narcotic drugs was carried out by simply comparing the mass spectra obtained by liquid chromatography tandem mass spectrometry (LC-MS/MS) with the pre-constructed in-house LC-MS/MS database of the existing narcotic drugs. Recently, a large number of newly synthesized narcotic drug structural analogue have been reported, which makes it extremely difficult to screen these illegal analogues through database searches. To effectively identify unknown narcotic drugs, we developed a screening software, AI-SNPS (Artificial Intelligence-Screener of narcotics and Psychotropic Substances), which consists of three layers, LC-MS/MS viewer, AI classifier, and identifier. In the AI classifier layer, classification of narcotic drugs can be carried out using artificial neural network (ANN), support vector machines (SVM) and K-nearest neighbor (KNN) models. Each model was constructed using a pre-selected training set (770 LC-MS/MS spectra), and these models classify the drugs into 13 different classes based on hierarchical clustering and fingerprint similarity calculations. The accuracy of the constructed model was evaluated using the external test set consisting of 193 LC-MS/MS spectra, in which the ANN, SVM and KNN models showed accuracy values of 75.1, 90.7 and 95.8%, respectively. The identifier layer uses pick-count scoring, simple similarity search, and hybrid similarity search (HSS) algorithms for the identification of narcotic drugs. In particular, the screening process using the HSS algorithm was carried out by shifting the peak in the database by delta mass (Δm) to match the precursor m/z value of an unknown substance in the acquired tandem mass spectra. Using abovementioned approaches, unknown analogues could be identified even when the database does not cover the targeted

substances. We believe that the developed AI-SNPS software would work as a powerful platform for screening unknown narcotic drugs and analogues. This research is funded by the Supreme Prosecutors' Office of the Ministry of Justice



Poster Presentation : **ANAL.P-429**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Liquid Chromatography/Mass Spectrometry of Marine Biotoxins with Simultaneous Screening and Identification by Product Ion Spectra

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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 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. Methods were optimized using commercially available reference standards such as gymnodimine-A, 13-desmethyl-spirolide C, pinnatoxin-E, F, G. Mixtures of CIs were separated according to hydrophobicity on C18 column and profiled by accurate molecular weight. Tandem MS (MS/MS) was performed while adjusting CID energy to generate an optimal fragment pattern for identifying CI types. 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 using newly developed analytical platform. This research was supported by a grant (20163MFDS64) from Ministry of Food and Drug Safety in 2021.

Poster Presentation : **ANAL.P-430**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Characterization of hetero-oligomeric cross-talk in Amyloid- β (1-42) using ion mobility mass spectrometry.

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Amyloid- β (1-42) has two additional hydrophobic residues at the C-terminal end compared to amyloid- β (1-40). In our previous study, we reported their fibrillation kinetics and structures at monomer level revealing the two peptides to have similar structural properties in solution phase, yet Amyloid- β (1-42) having focal localization of the radius of gyration distribution relative to Amyloid- β (1-40). Also taking account that homo-oligomerization was favored in Amyloid- β (1-42), it has been discussed that the two hydrophobic residues to contribute to the acceleration of hydrophobic clustering. Moreover, mixing of these two primary structure-similar peptides formed hetero-oligomers at early aggregation stage resulting in kinetical delay of the fibrillation process. Based on these previous observations, we designed a homologous peptide to delay fibrillation process by disturbing intramolecular hydrophobic interactions between peptides. In order to interrupt the self-assembly of wild type Amyloid- β (1-42) in the same manner, designed mutants should have similar structural properties to wild type at monomer level. Formation of the Amyloid- β (1-42) hetero-oligomer was monitored with ion mobility mass spectrometry. Structural analysis using multiple biophysical approaches, including circular dichroism (CD), solution phase small angle X-ray scattering (solution SAXS), and molecular dynamics (MD) simulation, provided insights into the molecular level mechanism of the cross-talk in Amyloid- β (1-42).

Poster Presentation : **ANAL.P-431**

Analytical Chemistry

Zoom 11 FRI 15:00~16:00

Development and Application of Liquid Handler for the Automated Pretreatment of TEMPO-FRIPS

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In analytic chemistry, robust and precise pre-treatment is essential for effective chemical reactions. Many commercial liquid handling robots have been developed to meet these needs, like reducing the laborious and time-consuming work. In this research, we devised a liquid handling robot suited for the TEMPO-FRIPS reaction by adopting the hardware of Opentrons OT-1. The parts for the framework, such as aluminum profile, Derlin V-slot wheel, belt, pulleys were purchased online. Some parts were fabricated by CNC machine, and other parts were 3D-printed. The geometry of the frameworks was optimized by trial and error. In the sense of software, the LabVIEW program was utilized to control a microprocessor, Arduino Due electronically. In the plan, we are planning to add vortex mixer, thermostat, centrifuge for the TEMPO-FRIPS reaction. After all functional parts are made, we will apply it to various of TEMPO-FRIPS experiments.

Poster Presentation : **ANAL.P-432**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Modification of Indium Tin Oxide with G6-OH PAMAM Dendrimer-Encapsulated Pt Nanoparticles for the Enhancement of Electrochemiluminescence

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In this study, we report surface modification of indium tin oxide (ITO) electrode with a hydroxyl-terminated polyamidoamine (PAMAM) dendrimer-encapsulated Pt Nanoparticles (hydroxyl-terminated Pt DENs) for improved electrochemiluminescence due to catalytic effect of the Pt DENs. Electrochemiluminescence (ECL) is a process in which species generated at electrodes undergo high energy electron transfer reactions to form excited states that emit light. ITO electrodes have features of good optical transmittance and excellent electrical conductivity, and are thus used to image electrochemiluminescence. However, there is limitation in that the electron transfer kinetics of ECL-related reactions at the electrode surface is low. Thus, methods of modifying the surface of the ITO electrode especially with catalytic nanoparticles to improve the kinetics are necessary to be studied. Based on this, it was reported that the ITO electrode could be modified with amine-terminated Pt DENs.¹ By modifying the surface of the ITO electrode with hydroxyl-terminated Pt DENs, we herein expand the types of catalysts, amine-terminated Pt DENs to hydroxyl-terminated Pt DENs, that can be grafted on the surface of ITO electrode for improved ECL.1. S. B. Lee, Y. Ju, Y. Kim et al., Chem. Commun., 2013, 49, 8913-8915

Poster Presentation : **ANAL.P-433**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Effect of the enhanced hydrophobic effect on structured and unstructured proteins in D₂O and H₂O.

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To avoid spectroscopic peak interferences such as H resonance frequency or O-H vibrational frequency in nuclear magnetic resonance (NMR), infrared (IR) spectroscopy etc., deuterium oxide (D₂O) is used as a solvent for a deuteration of sample molecules. Deuteration is used to avoid spectroscopic interferences, but it is controversial whether deuteration influences protein structures. Deuterium oxide (D₂O) is used at nuclear magnetic resonance (NMR), infrared (IR) spectroscopy as a solvent to avoid peak interferences, such as H resonance frequency or O-H vibrational frequency. Due to lower vibrational frequency of O-D (~1200 cm⁻¹) than that of O-H (~1600 cm⁻¹), D₂O is more stable than H₂O, with stronger hydrophobic effect. For this reason, there was a research that a globular protein is more stable in D₂O. But there is few researches about the protein structural changes or protein fibrillation mechanisms in D₂O. In this research, we used human insulin and α -synuclein to study the effect of reinforced hydrophobic effect on the structured proteins and IDPs' structures and protein stability-fibrillation. In addition, the experiment was further carried out under conditions of structural denaturation by adding sodium dodecyl sulfate (SDS), a protein denaturant, to insulin. 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-434**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

NMR Structural Studies of Anti-inflammatory effect of tIK peptide

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Rheumatoid arthritis is an autoimmune disease in which inflammation occurs in the synovial membrane around the joint, destroying ligaments and cartilage. This inflammation spreads to blood vessels and skin, causing anemia, headache, and vasculitis. An imbalance between pro-inflammatory and anti-inflammatory cytokines is known to be one of the causes of this disease. Recent studies have shown that the truncated-IL-10 (tIK) protein inhibits the expression of inflammatory cytokines. Therefore, we conducted research to develop anti-inflammatory peptides based on the tIK sequence. Phosphorylation patterns in macrophages of tIK transgenic mice were investigated, and tIK protein phosphorylated the 496th tyrosine of the interleukin (IL)-10 receptor subunit alpha to have anti-inflammatory effects. In order to find a specific sequence of tIK protein that induces phosphorylation of IL-10 receptor, the structure of tIK was predicted using sequence homology modeling with IL-10 and four epitopes were proposed. The anti-inflammatory activity of each epitope was confirmed by the TH17 cell differentiation test, and the peptide consisting of 18 amino acids with the best anti-inflammatory effect was named tIK 18-mer. Based on this, 9mer and 14mer, which have anti-inflammatory effects, were also found. Peptide expression was performed with E.coli, confirmed that it was successfully performed through MALDI-TOF and NMR, and the experimental procedure was optimized. The secondary structure of the peptide was confirmed by 2D NMR and CD, and chemical shift perturbation was studied to elucidate the interaction between the anti-inflammatory peptide and the receptor. Finally, anti-inflammatory tests of the peptides were conducted to confirm the anti-inflammatory effect of the purified peptide.

Poster Presentation : **ANAL.P-435**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Improved MALDI-MS Detection of Semiconductor Nanocrystals Using Porphyrin Matrices

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Mass spectrometry is widely used analytical method to study nanoparticles (NPs), providing useful information about their masses and compositions. Especially, matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) has been applied to studies of various NPs including quantum dots (QDs). However, since most of NPs struggle for the ionization, increasing ionization efficiency is one of critical issues to be solved in the study of NPs using MS. When NPs are investigated by MALDI-MS, this ionization efficiency is highly dependent on the choice of matrix required to support ionization process. Despite of the importance of matrix, previous mass studies of NPs were mainly progressed using *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene] malononitrile (DCTB) as a matrix. In the present work, we investigate the ionization efficiency of QDs with several matrices based on MALDI-TOF instrument. Interestingly, compared to other conventional matrices, QDs with porphyrin-based matrices showed remarkable improvement in intensity on the mass spectrum regardless of types of QDs, indicating increase in electron transfer. Enhanced intensity on mass spectrum is possibly explained with the new ionization mechanism based on properties of QDs and electron acceptor matrix. Porphyrin-based matrices, as both good electron donors and acceptors, are expected to deprive electrons from excited QD better than conventional matrices, resulting in higher electron transfer efficiency. Additional to the experimental MS data, fluorescence tests of several NPs with and without matrix are ongoing to further support the role of electrophilic matrix in ionization process of QDs.

Poster Presentation : **ANAL.P-436**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

NMR Structural studies of antimicrobial peptides, Lactophorin

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Antimicrobial peptides (AMPs) solve the problems of existing antibiotics, and many studies have been conducted as a novel kind of antibiotic. The AMPs studied in this research are analogs of Lactophorin-I (LPcin-I). Proteose-peptone component-3 (PP3) is a hydrophilic phosphorylated glycoprotein, which is involved in the physicochemical properties of proteose-peptone and plays an important biological role in cow milk. The 113-135th region of the C-terminus of PP3 is called LPcin-I, which is a cationic amphiphilic antimicrobial peptide. LPcin-I has antimicrobial activity against Gram-positive and Gram-negative bacteria, but it is known that it does not cause hemolysis of human erythrocyte. Through peptide engineering based on LPcin-I, candidate peptides which have improved antimicrobial properties against LPcin-I were selected. At this time, YK3 showed the best antimicrobial activity, and based on this, a shorter length of AMPs were developed by peptide engineering. Based on YK3, novel AMPs were designed and that their structure and antimicrobial activity were to be confirm. In order to express the LPcin analogs in large quantities, a gene recombination method was used, and a high purity isolation and purification method was optimized. The orientation and structure of the analogs bound to the lipid double membrane was confirmed using CD, solution/solid-state NMR spectroscopy. In particular, solution-state NMR can measure the secondary structure, orientation of proteins in biologically appropriate lipid double membranes. Using solid-state NMR, it is possible to identify topology and study its mechanism of antimicrobial activity. For solid-state NMR studies, a solid NMR probe for ¹H-¹⁵N measurement and ¹H-³¹P measurement were manufactured in our laboratory.

Poster Presentation : ANAL.P-437

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Analysis of photothermal effect with different size of Bi-Te Covered Nanorods on 2D monolayer and 3D spheroid neuroblastoma cells

Chae ri Park, MyungKook Son, Dongjoon Im, Sooyeon Chae, Dongvin Kwak, Hugh I. Kim*

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

Poster Presentation : **ANAL.P-438**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Disease-related transmembrane protein by Solution & Solid-state NMR Spectroscopy

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Human transmembrane proteins (hTMPs) are playing an important role in the biological system like gateways to permit the transport of a specific substance. It is associated with various diseases, which can lead to loss of function and signal transmission system errors as a substance carrier. Since the function of a protein is closely related to its structure, it is important to clearly know the structure of the protein. However, with the innate insolubility of TMP, it is seriously difficult to prepare the sample of TMP. The human melanocortin-4 receptors (hMC4R), which play an important role in appetite control and energy homogeneity, are valuable because they are directly related to presenting genetic problem-solving directions for human obesity. A mutation in hMC4R replacing the 90th amino acid with asparagine located in the second transmembrane domain (TM2) was found in patients with early onset-obesity. Alzheimer's disease is related to the transmembrane domain of amyloid precursor proteins (APP-TM). To explain more details, the APP-TM forms an ion channel that Ca²⁺ permeability in the cell membrane, destroying calcium ion homeostasis in a normal cell. The Syndecan-4 (Syd4) performs various functions such as cell-to-cell interaction, extracellular matrix interaction, cancer progression, cell proliferation. To know the structural characteristics, wild type Syndecan-4 TM (wtSyd4) and mutant Syd4 TM (mSyd4) which is the gene that mutated GxxxG motif was expressed and purified. In this study, to obtain highly purified protein, the expression and purification process were optimized. After that, we employ diverse analysis techniques such as PAGE, CD, MS, solution/solid-state NMR spectroscopy to analyze the highly purified proteins through optimized experiment.

Poster Presentation : **ANAL.P-439**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Nanoparticle Size Determines the Affinity of High-Density Lipoprotein Particles for Pegylated Gold Nanoparticles in Biomolecular Corona Formation

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When nanoparticles come in contact with the biological fluids, some of biomolecules, especially proteins, immediately adsorb on the surfaces of nanoparticles, which leads to protein coronas. It has been known that protein coronas play an important role in the biocompatibility of nanoparticles, and precise understanding of interaction between nanoparticles and biomolecules is critical for nanomaterials safety. In this study, various analysis techniques were utilized in a combined way to understand the properties of protein coronas, which included TEM, nanoparticle tracking analysis, UV-VIS spectrophotometry, and gel electrophoresis. Using the techniques, formation of biomolecular coronas of high-density lipoproteins (HDLs) on the pegylated gold nanoparticles of various sizes (20 – 150 nm diameter) were investigated quantitatively, which revealed an explicit increase in the affinity of HDLs for less-curved nanoparticle surfaces, further suggesting that the adsorption is initially governed by the particle nature of HDLs rather than its constituent biomolecules such as apolipoproteins.

Poster Presentation : **ANAL.P-440**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Investigating the deteriorated drug efficiency of cisplatin induced by DMSO using ICP-MS

Dongvin Kwak, Hugh I. Kim^{*}, Sooyeon Chae, MyungKook Son, Dongjoon Im, Chae Ri Park

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Cisplatin (cis-[Pt(NH₃)₂Cl₂]) is a platinum-based anticancer drug used for diverse cancers. Because of acquired or intrinsic resistance against to cisplatin, a large number of in vitro studies have been conducted to clarify the mechanism of this phenomena. In most of these studies, dimethyl sulfoxide (DMSO) has been utilized as solvent for the stock solution of cisplatin. According to a study concerning effects of solvents on the activity of cisplatin, DMSO depresses cytotoxic efficiency via ligand exchange with Cl⁻. However, very few studies have been published on which steps DMSO affects on. The steps is divided into 1. Passive diffusion/transportation through cell membrane/transporters 2. One or two Cl⁻ ligands are exchanged with H₂O due to low [Cl⁻] in cytoplasm resulting active form 3. Active forms of cisplatin coordinate mainly to N(7) of guanine, adenine 4. DNA kink induced by Pt coordination leads cell apoptosis signalling pathways. In this study, we investigated which steps exactly are affected by DMSO solvent.

Poster Presentation : **ANAL.P-441**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Investigation of Mechanisms and Drug Uptake in Human neuroblastoma SK-N-SH Cells in 3D Spheroids

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Neuroblastoma is an uncommon pediatric cancer and to be diagnosed in the first year of life. It is a complex and heterogeneous disease therefore many factors, such as age, gene mutation, cell differentiation level, and stage of disease, affect therapeutic diagnose. As neuroblastoma belongs to heterogeneous disease, cancer cells can show distinct morphological and phenotypic profiles including cellular morphology, gene expression, metabolism, motility, proliferation, and metastatic potential. To maximize treatment efficiency, tailor treatment is applied to each patient. However, it is still challenging because of complexity of disease and the different response between 2-dimensional (2D) model system and real tumor. 3D spheroids of tumor cells can reflect the characteristics of solid tumors by retaining cell-cell interactions and microenvironments such as hypoxic conditions that better reflect drug resistance than 2D models. This model system can provide more comprehensive information about the preclinical drug response of neuroblastoma cells inside the solid tumor. Several studies approach to explore the differences in 3D spheroids and 2D cells. However, it is still challenging to understand differences in morphology and microenvironments in 3D spheroids compared to those in 2D monolayers that influence the drug response and the mechanisms of action. In this study, we investigated the pathology mechanisms and drug uptake in SK-N-SH neuroblastoma cells cultured in 3D spheroids compared to those in 2D monolayers using electrospray ionization mass spectrometry (ESI-MS) and computational fluid dynamics.

Poster Presentation : **ANAL.P-442**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Elucidation of PL Property of Au Nanoclusters by Interaction with Pb²⁺ and Cu²⁺ Ions

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Metal nanoclusters (Au, Ag, Cu, etc.), which composed of several to hundreds of metal ions, have been received significant attention owing to their strong quantum confinement effect. In particular, Au nanoclusters (Au NCs) have attracted tremendous interest because of their wide range of applications in catalysis, sensing, bio-imaging, and so on. However, the use of fluorescent Au NCs is still not competitive in practical applications than QDs and organic dyes because of the lack of full understanding of the origination of PL property of Au NCs. So far, two main approaches to explain the PL property of Au NCs have been developed, i.e., metal quantum confinement effect and charge transfer effect. These are still debating but, the latter one has accepted as a more reasonable approach. For example, the PL property of Au NCs is strongly variable depending on the type of capping agent, and it depends strongly on the types of metal ions when the Au NCs interact with metal ions. These are good examples to explain the charge transfer mechanism between the metal core and capping agent. In this study, we have elucidated the change in PL property from the point of view of the change in the surface state of Au NCs by interaction with Pb²⁺ and Cu²⁺ ions. Consequently, we found that the photoinduced charge transfer (PCT) is predominant for the case of Pb²⁺ ion but, the photoinduced electron transfer (PET) is the more favorable route for the case of Cu²⁺ ion.

Poster Presentation : **ANAL.P-443**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Structural elucidation of glycoconjugates in humanized mouse liver tissue using LC-MS/MS

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Mouse is the most common model in the preclinical test and liver tissue is used to test the drug metabolism and prediction of in-vivo kinetics. Drug metabolism is an important issue in preclinical test for produce more safe and effective candidates. However, the general success rate of new drug candidates during clinical trials is still low. One outstanding explanation is difference of glycosylation, in which inter-species differences between the mouse models and humans. Recent studies have shown that two critical differences (Neu5Gc, alpha-gal) have been identified between humans and other mammals. Especially, Neu5Gc epitopes could lead to several inflammatory disorders. Also, alpha-gal is known to cause of severe hypersensitivity reactions after xenotransplantation. For this reason, "humanized" mouse models such as triple-knockout (CMAH/GGTA1/iGb3S) models related to Neu5Gc and alpha-gal epitopes have been developed. However, there is still lack of the study on qualitative and quantitative glycoconjugates structure details. Here, we elucidated the structure of glycan and glycolipids obtained from mouse liver tissue by LC-MS/MS in both negative and positive ion detection mode. Negative ion mode MS/MS provides sensitive detection sialic acid-containing structures with lower background noise whereas positive mode MS/MS produces more detailed lipids fragment ions such as ceramide. The analysis data demonstrated the presence of known Neu5Gc and alpha-gal antigens. Furthermore, we could identify differently glycosylation, between humans and mouse such as sialylated HexNAc, unique Neu5Ac-containing N-glycan, co-existence of NeuAc and NeuGc containing N-glycan. Finally, this structure information provides a reference to other new potentially functional glycan structures.

Poster Presentation : **ANAL.P-444**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Real-time Monitoring Growth of Single Bacteria using Droplet-based Microfluidics and Identification of Bacterial Gas Metabolism in Microenvironment

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Droplet-based microfluidics (DMF) has been developed in analytical chemistry to analysis chemical and biological components such as viruses, bacteria and nucleic acid. Generation of monodisperse droplets is important for the accurate and sensitive analysis where droplets must be kept in stable for various applications including single-molecule detection and droplet digital PCR. To guarantee stability of droplets, droplets are normally generated with oil and surfactant. Among various surfactants, PFPE-PEG-PFPE surfactant demonstrated have been widely used in DMF that surfactant was introduced from Weitz group because of stability and biocompatibility. However, there are no studies on gas crosstalk between droplets. Therefore, we experimentally confirmed that gas crosstalk occurred between droplets. *E. coli* K-12 cells were encapsulated within droplets for the cultivation, and gas crosstalk was identified with neighboring droplets that contain the phenol red. Since bacteria produce ammonia gas during cultivation, penetration of ammonia gas initiates a color change of phenol red-containing droplets. Ammonia gas was artificially produced through a chemical reaction between ammonium chloride and sodium hydroxide within droplets to experimentally confirmed that the ammonia gas can transport into neighboring droplets. We also confirmed that surfactant density affects the gas permeability between droplets. In this study, it was verified that crosstalk of ammonia gas, a bacterial metabolite, was occurred between droplets encapsulated by PFPE-PEG-PFPE surfactants. Our results suggest that DMF can be used for monitoring of living bacteria by bacterial metabolites and this phenomenon can be applied for microenvironmental chemical reaction that required gas as catalysts.

Poster Presentation : **ANAL.P-445**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Comparison of thermal desorption (TD) sorbent tubes with SPME fibers for the analysis of combustion gases from fossil fuels

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The characterization of combustion gases from fuel oils is important for the identification of cause of fire and investigation of arson suspects. In this study, we combusted three kinds of fuel oils such as diesel, kerosene, and gasoline refined by three different refinery companies, for which combustion gases were characterized using TD/GC-MS and SPME/GC-MS. For the comparison purposes, two TD sorbent tubes (Tenex® TA, and Airtox™) and four SPME fibers (PDMS, PDMS/DVB, CAR/PDMS, and DVB/CAR/PDMS) were utilized for gas sampling. The results showed that two different sampling methods have comparable absorption efficiencies. In addition, three different TD sorbent tubes and fibers showed different compatibility to the type of fuel oils. It was found that Airtox™, CAR/PDMS, and DVB/CAR/PDMS are suitable for the adsorption of combustion gases from kerosene and diesel. Tenex® TA and CAR/PDMS showed high adsorption compatibility for gasoline. On the other hand, Airtox™ was found to be the most appropriate adsorption tube for relatively light gases under 130 Da.

Poster Presentation : **ANAL.P-446**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Effect of Cobalt Salts and Reducing Agents for Cobalt Nanoparticle Formation in Aqueous Solution

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The liquid phase reduction method is synthesizing metal nanoparticles at room temperature and pressure. In this process, metal particles have different shapes and sizes depending on the reagents. Here, we fabricated cobalt nanoparticles by reducing the cobalt salt, CoCl_2 , CoBr_2 , $\text{Co}(\text{NO}_3)_2$ in the CTAB aqueous solution. At this time, it was confirmed in what form the reaction was performed depending on the cobalt salt used. Also, we used NaBH_4 and hydroquinone as the reducing agents that were used to synthesize the gold nanoparticles in the previous study. The Optical Properties of the nanoparticles were measured by UV-Vis spectrum, and the shape was measured through SEM image analysis.

Poster Presentation : **ANAL.P-447**

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Quantitative Analysis in Proteomics using ^{18}O Labeling on Target Proteins and Unlabeled Standards

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A new strategy called QAUSIA (Quantitative Analysis using Unlabeled Standards and Isotope-labeled Analytes) was proposed for the use of such unlabeled standards and labeled analytes in absolute quantitative analysis in proteomics by mass spectrometry. A procedure with repeated ^{18}O labeling was adopted to produce such ^{18}O -enriched peptides for investigation of labeling efficiency, response factor, and calibration curve. Calibration curves employing unlabeled peptide as internal standard showed good linearity and similar slopes calculated from both mass spectrum and the extracted ion chromatogram. Subsequently, the QAUSIA strategy was tested using the target peptide of ovalbumin, and the calibration slope obtained from QAUSIA using the unlabeled synthetic peptide as a standard showed very similar results to the AQUA-based analysis. In addition, the concentration of the QAUSIA strategy using the targeted peptide of ovalbumin was 5.07 ± 0.14 nmol with respect to the theoretical expected value of 5.02 nmol, showing excellent accuracy.

Poster Presentation : ANAL.P-448

Analytical Chemistry

Zoom 11 FRI 16:00~17:00

Characteristics and Electrochemical Performances of Carbon nanofibers/Transition Metal/nano-Silicon Composites as Anode Material for Lithium Secondary Batteries

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Silicon (Si) has been considered as the next generation ideal anode material for lithium-ion batteries because of its highest theoretical capacity ($4,200 \text{ mAh}\cdot\text{g}^{-1}$) and affluent reserves in nature. However, the severe volume expansion and unstable solid electrolyte interface (SEI) film of Si electrode during lithiation/delithiation, as well as the poor electron conductivity have seriously restricted its commercial application. In this study, transition metal coated silicon was synthesized and applied as anode materials of Li secondary batteries. The transition metal salts of Fe, Ni, and Cu were dissolved in aqueous solution and used to coat metals on the silicon nanoparticles. The transition metal coated silicon was simply modified by electroless plating method. Coating was achieved by dropwise the metal solutions in silicon solutions. Carbon nanofibers (CNFs) were then grown on the transition metal coated Si nanoparticles and these composite materials were applied as anode materials for Li secondary batteries. The morphologies, compositions, and crystal quality of transition metal/silicon composites were characterized by scanning electron microscopy (SEM), Raman spectroscopy (Raman) and X-ray photoelectron spectroscopy (XPS). The electrochemical characteristics of CNFs/transition metal/silicon composites as anodes of Li secondary batteries were investigated using a coin cell and battery tester.

Poster Presentation : **LIFE.P-449**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Development of Immunoglobulin G delivery vehicle at Nanomolar concentrations with Domain Z-fused Multimeric α -Helical Cell Penetrating Peptides

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Antibody is supreme recognizing machinery in nature. Because of their high selectivity and sensitivity, they have been widely used for therapeutic, diagnostic tools and biological research tools. Although they are very useful for various fields, most antibody applications are limited to the cell exterior due to their impermeability into live cell membrane. Therefore, efficient antibody delivery vehicles are still needed to be developed. Here, we introduce a new vehicle designed for the intracellular delivery of antibodies into live cells at nanomolar concentrations using domain Z, the affibody targeting Fc regions of immunoglobulin G (IgG), and the multimeric LK sequences, the powerful cell penetrating peptide. The LK-domain Z can non-covalently bind with IgG at specific ratio by simple mixing and cell permeable IgG/LK-domain Z complexes are created. The IgG/LK-domain Z complexes successfully penetrate live cells at nanomolar concentrations and the delivery efficiency is strongly dependent on the concentrations of the complex. The complexes penetrate cells via ATP-dependent endocytosis pathway and we confirmed that most of delivered IgG can escape from endosome to cytosol. Furthermore, we believe LK-domain Z can be used as a future therapeutic tool, as we successfully controlled the targeted intracellular signaling pathway related to tumor proliferation by delivering anti-NF- κ B using LK-domain Z vehicle with a cathepsin B-cleavable linker between LK and domain Z. This newly found IgG vehicle is expected to facilitate various biological studies and development of new future therapeutics.

Poster Presentation : **LIFE.P-450**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Design of self-assembled catalysts with amyloidogenic peptides

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Amyloid is a supramolecular fibril composed of thousands of mono-peptides. Through intermolecular hydrogen bonding, β -sheets are oriented perpendicularly to the fiber axis. Amyloid fibers are known to involve in pathological conditions. However, recent studies discovered that amyloid fibers provide beneficial functions to living organisms. These amyloid fibers are also called functional amyloids. Functional amyloids can be found in numerous organisms such as fungi, bacteria, insects, and even humans. The amyloid structure can offer advantages to organisms due to its unique characteristics to form supramolecular structures from simple monomers through self-assembly. There are examples utilizing these properties to design self-assembled catalysts with amyloidogenic peptides. We synthesized a short peptide (Ac-IHIHIYI-NH₂; Ac-Y) through the solid phase peptide synthesis method. Ac-Y contains two histidine residue to bind with copper(II) ions. Due to the intrinsic redox activity of a copper ion, when peptides are bound with copper(II) ions, they can also promote redox reaction. Through this work, we showed that Ac-Y bound to copper(II) ions has a synergistic catalytic effect on the oxidative association of dopamine, also known as the formation of melanin-like species.

Poster Presentation : **LIFE.P-451**

Life Chemistry

Zoom 21 FRI 16:00~17:00

pH-dependent modulation of RPT via liquid-liquid phase separation (LLPS)

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Intrinsically disordered proteins/peptides (IDPs) are spontaneously organized into phase-separated liquid droplets, which is also called coacervation (FUS, P granules, etc). In general, IDPs have a low sequence-complexity and are rich in A, G, R, T, S, K, Q, E, P. Remarkably, proteins having pH-responsive behaviors often exhibit some characteristics of IDP, with other dynamic properties. We sought to use repeat-domain (RPT) of premelanosome protein 17 (Pmel17) to identify its phase-separation behaviors. A number of experiments focused on recognizing the presence and characteristics of the coacervation of RPT depending on pH have been conducted. RPT at lower pH(3~5) formed coacervates rapidly, which became gel-like aggregates within 12 hr. Turbidity assay suggested that such an aggregation process was similar to previously reported two-phase amyloidogenesis. On the other hand, medium pH (6~8) led to the delayed coacervation of RPT, which, interestingly, was stable in the coacervation state for more than two weeks. Potential functionality of the stable RPT coacervates in melanogenesis was also investigated.

Poster Presentation : **LIFE.P-452**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Microwave-Assisted Solid Phase Peptide Synthesis (SPPS) & Cysteine modification

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In this research, we are optimizing automatic peptide synthesis system for designing peptide library composed of various isotope-labeled signal peptides, which are considered to be related to the tumor development research. Isotope-labeled signal peptides are straightforwardly synthesized by utilizing a powerful tool, microwave-assisted solid phase peptide synthesis (SPPS), which enables various peptides to be synthesized in high speed and high efficiency. Through the isotope-labeled peptide library and their mass spectrometry analysis, the database of tumor-associated peptides is being constructed, which we expect to contribute to clarifying the major causes of cancer on a molecular scale and reducing the diagnosis time for cancer. However, we are confronted with several critical issues concerning cysteine-containing peptides. First, due to the susceptibility of cysteine to epimerization, cysteine-containing peptide shows relatively low yield and high impurities in microwave-assisted SPPS, compared to other ordinary peptides. Second, cysteine, whose side chain is sulfhydryl group, is liable to form disulfide bridges among peptide chains. Since the formation of disulfide bond severely interrupts precise analysis of LC/MS/MS, the sulfhydryl group should be capped through reduction or alkylation, not only to prevent the formation of disulfide bond but also to cleave disulfide bonds prior to the LC/MS/MS analysis. However, it is being issued as a serious problem that excessive alkylation in peptide synthesis is also observed by LC/MS/MS analysis. In this poster, we present the synthesis of cysteine-containing peptides and the optimized reaction conditions to suppress the side alkylation reaction of cysteine-containing peptides.

Poster Presentation : **LIFE.P-453**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Melanogenesis inhibitory activity of *N*-trans-caffeoyltyramine isolated from hemp seed ethyl acetate fraction

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Melanin is a pigment that provides coloration and plays an important role in protecting human skin from harmful effects of UV light radiation. However, dysregulation in melanin synthesis causes several skin problems including freckles, melasma, age spots and other hyperpigmentation syndrome. Tyrosinase is one of the key enzymes in melanin synthesis. It is an oxidase and rate-limiting enzyme for controlling the production of melanin. Therefore, down-regulation of enzyme activity is the most efficient method for the inhibition of melanogenesis. Hemp seed has beneficial effects on human health. Because it has essential amino acids, unsaturated fatty acids, various minerals and vitamins belonging to B family, which are not produced in human body. In this study, we prepared hemp seed extract and its solvent fractions and evaluated their biological activity against free radical and melanin synthesis. Defatted hemp seed extract has better tyrosinase inhibition activity and ABTS radical scavenging activity than fat extract *in vitro*. The defatted extract inhibited tyrosinase activity *in vitro* more efficiently than arbutin. Comparative evaluation of radical scavenging and anti-tyrosinase activity of hemp seed solvent fraction showed that the ethyl acetate fraction has the highest potential for inhibition of melanogenesis. We used high-performance liquid chromatography (HPLC) and NMR spectroscopy for structural analysis. As a result, we found that one of the compounds contained in the ethyl acetate fraction was *N*-trans-caffeoyltyramine. It has an inhibitory effect on α -MSH-induced melanogenesis. In conclusion, *N*-trans-caffeoyltyramine or ethyl acetate fraction of defatted hemp seed extract might be useful in cosmetics as a skin-whitening agent.

Poster Presentation : **LIFE.P-454**

Life Chemistry

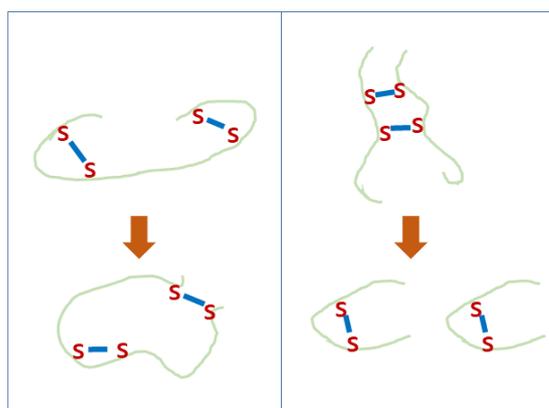
Zoom 21 FRI 16:00~17:00

An Alternative Production of Recombinant Proteins Containing Disulfide Bonds in *E. coli*.

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The disulfide bond formation is an important post-translational modification because they not only increase the structural stability of the protein, but can also play a catalytic role in the redox reactions. However, proteins with more than two disulfide bonds are difficult to make in *E. Coli* by the recombinant fashion. This is because they mostly form inclusion bodies due to the wrong folding or the mismatch of two non-native pair of cysteines, through either intra- or intermolecular bonding. People have developed several methods, but the success rate is rather low yet. For a protein that is readily refoldable, people try to start from and refold the inclusion bodies. For a lot more other proteins that cannot be refolded *in vitro*, people can try: (1) the specialized strains such as Origami or Rosetta-gami in which the two proteins, thioredoxin and glutaredoxin, are not produced, so the already formed disulfides remain oxidized, and/or (2) the coexpression of Dsb or PDI proteins which can catalyze the formation of disulfides. Our lab aims at producing native/soluble disulfide containing proteins. We have developed and accumulated data from two techniques. They were developed separately, but we combined them, and we are now seeing a breakthrough in this predicament. The auto-induction component helps prepare cultures in the slowly growing condition (at low temperature and/or under environmental stresses). The metabolite profiling data under stresses provide guidance how to apply which stress to better make soluble proteins. The great advantages of these steps are that any special or sophisticated material or machine is not needed, and the screening can be carried out in a high throughput fashion. This research was supported by NRF-2018K2A9A1A06065371.



Poster Presentation : **LIFE.P-455**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Development of a combination therapy for STING agonist elevating immune response

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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' by stimulation of innate immunity. The natural ligand for STING, such as 2'3'-cyclic GMP-AMP(cGAMP), or synthetic cyclic dinucleotide(CDN) type of STING agonists activate IFN-mediated immune response and promote anti-cancer immunity. Despite the promising pre-clinical outcome, CDN derivatives are limited in clinics due to the narrow application via IT administration and unfavorable pharmacokinetic properties. Therefore, there exists continuous effort to develop a combination therapy with synergistic effect for STING agonists. Here, we report a new compound bearing indolizine as a pharmacophore that enhanced cGAMP-induced type I IFN innate immune response by increasing phosphorylation of IRF3 in the downstream signaling pathway of the STING-TBK1 complex.

Poster Presentation : **LIFE.P-456**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Collagen Fibrils Formation from Collagen-encapsulated Nanoliposomes using Electrical Stimulation

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Collagen is one of the prominent scaffolding components of the extracellular matrix that can turn into collagen fibers through self-assembly mechanisms. Recently, we found that an electric field can stimulate the collagen fiber formation process in an acidic condition through the migration and aggregation of tropocollagen. When applying an AC of 10Hz-1V, collagen fibrils with a 28 to 70 nm diameter appeared within 9 minutes in a 0.01M HCl pH three solution. Further, we designed an experiment to form collagen fiber by encapsulating collagen molecules in nano-sized liposomes (Lip-Col) and confirmed that the fibrils could be formed from Lip-Col in the same condition. First, we filtered the collagen solution through a polyethersulfone membrane and measured the average particle size, encapsulation efficiency, and stability of Lip-Cols at various pH conditions. Under the electric field, Lip-Cols started to aggregate and align into collagen fibrils after 3 and 13 minutes, respectively. Fluorescence imaging results showed that collagen fibrils were formed in a matrix-like structure and could enhance the biosynthesis of collagen type I in human dermal fibroblasts. Based on these findings, these Lip-Cols can be utilized as a drug delivery system for anti-aging or wound healing agents.

Poster Presentation : **LIFE.P-457**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Artificial cellular model for actin-membrane interactions with controlled actin polymerization

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In a cellular system, both the cytoskeleton and the membranes are under dynamic and complex networks to maintain 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 for further understanding the cellular bioactivities. Here, 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 GUVs had Mg²⁺ ionophores embedded, enabling Mg²⁺ to travel this model's inner condition, which triggered polymerization. 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-458**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Morphological changes of artificial cell: cholesterol effects on controlled microtubule polymerization in a giant unilamellar vesicle

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The cytoskeletons, including microtubules, are of crucial importance in a cellular system for controlling huge aspects of cell morphologies and shape change. In particular, these bio-compartments' spatial organization in a cell-mimicking boundary has lately drawn much attention in that constraints imposed by confined areas would be likely to give more of an in-vivo structure of those components. However, recent studies over cytoskeletons in vesicles have been mostly limited to actin, and a few types of research on microtubules were only conducted in lipid monolayer droplets, not liposomes. Herein, we constructed an artificial cellular model that explains several variations of cytoskeletal networks between self-polymerizing microtubules and bilayer membranes that are differently conditioned with cholesterol ratio and saturation of lipids. The giant unilamellar vesicles (GUV) had magnesium ionophores embedded, enabling Mg²⁺ to travel the lumen of this spherical model, which finally triggers the polymerization. As tubulin filaments grew in GUVs, they resulted in different spatial organization inside the vesicle, depending on the cholesterol and saturated level of lipids. Some tubulin dimers were bound to unsaturated lipids, and cholesterol had microtubules grow toward the membrane, being attracted to them. Our models are the closed system that shows the possibility of creating artificial cellular morphology changes with only the interactions between cytoskeletal proteins and membranes with controlled microtubule polymerization.

Poster Presentation : **LIFE.P-459**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Identification of differential expression genes(DEGs) in groups before and after molting of long-tailed chickens

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RNA-Sequencing(RNA-Seq) technology is an essential high-throughput sequencing technology for analyzing transcripts of all organisms, and measures changes in gene expression such as gene function, alternative splicing, and gene expression differences. In addition, since differential expression analysis for comparison of expression between groups is possible, it is possible to analyze which genes show differences in RNA-Seq data with gene expression measurement software such as cuffdiff, DESeq, and edgeR. In this study, differential expression analysis was performed to find differential expression genes(DEGs) showing differences in gene expression in groups before and after molting of female long-tailed chickens. The quality of the RNA-seq read was confirmed with the FastQC program, and mapped with the reference file using TopHat2. After assembly into a series of transcripts via cufflink, we compared the relative amounts of mRNA using cuffdiff, and then set the absolute value \log_2 fold change ≥ 1 , p-value

Poster Presentation : **LIFE.P-460**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Screening of natural product compounds which stimulate CYP11A1 expression as anti-kidney cancer drug candidates

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The incidence of Renal cell carcinoma (RCC) differs widely in various parts of the world, approximately 403,000 new cases of RCC along with 175,000 deaths because of kidney cancer in 2018. Early diagnosis while cancer is still localized increases the rate of survival and gave better chance to overcome the disease. CYP11A1 is a mitochondrial side-chain cleavage enzyme which are involved first step of steroid synthesis and associated downregulate in various cancer types. Furthermore, the deficiency of CYP11A1 can cause adrenal insufficiency that lead to lethal when untreated. Our study presents a broad to determine whether CYP11A1 impair the migration of cancer cell, we investigated the effects of inhibition and activation of CYP11A1 enzymatic activation using the inhibitor - Aminoglutethimide and the activator - Mitomycin C. In this context, we screened a panel of natural product compounds from Korea Chemical Bank with model of CYP11A1 overexpressed in Caki-1 cell line. In vitro modeling showed the inhibition of cancer cell migration consistent with its activation of CYP11A1. We identified several potential natural product compounds show their stimulation effect to CYP11A1. Further experiment will be conducted to evaluate changing in quantification of steroid hormones level by Multiple Reaction Monitoring (MRM) based LC-MS/MS approach. The findings of the present study might suggest newly therapeutic target and anti-cancer drug candidate occurring especially for kidney cancer.

Poster Presentation : LIFE.P-461

Life Chemistry

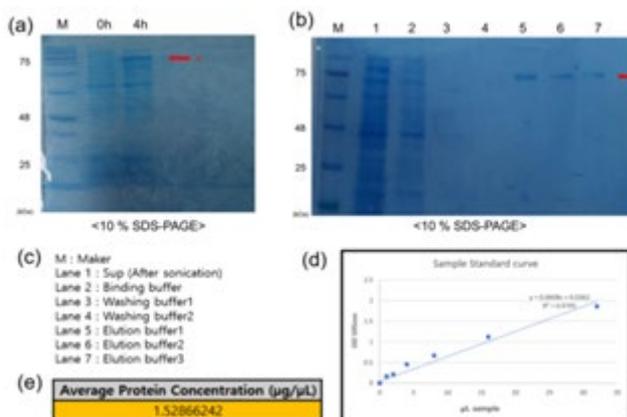
Zoom 21 FRI 16:00~17:00

Identification of expression and purification about Visfatin.

Choi Bo Hee, Jang-su Park*

Department of Chemistry, Pusan National University, Korea

1. Introduction Visfatin binds to a fixed-phase bead within the Ni column, and proteins that do not bind to ligand are washed by spilling with a column buffer solution. Proceed with Binding buffer, Washing Buffer, and Elution Buffer of Sup and pass each solution through the column in the Nickel column. Absorb the Nickel column with the Sup Binding and lower the Binding so that the protein sticks well to the column. In the Washing Buffer, remove all except the protein that I want to obtain from the Ni column. Due to the difference in the concentration of Immidazole, proteins other than Ni column and Visfatin, which have high efficiency, are eluted with the wash buffer. Finally, the remaining Visfatin in the Ni column is collected through the Elution Buffer using a high concentration immidazole. 2. Material & Conclusion a) After the injection of IPTG, the protein sample of 0h 4h can be dropped on the SDS PAGE gel to confirm that the band that was not in 0h was created after 4h. This shows that Visfatin has been expressed. (b and c) (d) OD595 was measured to measure the composition of the protein, and a graph was drawn and a trend line was drawn. (e) The measured values of average Protein Concentration (mg/mL) Also GFP tags shows that visfatin has been expressed.



Poster Presentation : **LIFE.P-462**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Verifying functional pathogenicity of Alzheimer's Disease related mutation

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Department of Bionano Technology, Gachon University, Korea

Background: Amyloid precursor protein (APP), presenilin1 (PSEN1), and presenilin2 (PSEN2) are considered to be pathological mutations in Early-onset Alzheimer's disease (EOAD). Among them, PSEN1 was found largest number of pathological mutations, which is a subunit of gamma secretase in processing APP to amyloid-beta ($A\beta$). Previously, PSEN1 Gly417Ala was found from a 37-year-old Korean male patient. Clinical manifestations presented memory deteriorations for over three years and was diagnosed with EOAD with mild symptoms of Parkinson's disease. To further establish the gene's implications in the pathology, a stable cell-line of PSEN1 Gly417Ala was produced by using CRISPR/Cas9 technology protocol to investigate its functional pathogenicity. Materials and Methods: HEK293 cells was transfected with gRNA of PSEN1 Gly417Ala by CRISPR/Cas9 technology. Functional study was performed using ELISAs of $A\beta_{40}$, $A\beta_{42}$ and $A\beta$ oligomers by Multiple Detection System (MDS). The gamma and beta secretase activities were measured by employing their specific substrates. Results: Successful transfection of PSEN1 Gly417Ala was confirmed by the restriction enzyme and sanger sequencing. Ratio of $A\beta$ and levels oligomers were elevated in PSEN1 Gly417Ala in comparison with control cells. Functional studies also indicated the elevated activities of both gamma secretase and beta secretase in PSEN1 G417A. These results may elaborate the pathogenic gene of PSEN1 G417A in Alzheimer's disease. Conclusions: CRISPR/Cas9 technology is a powerful tool in studying the pathogenicity of PSEN1 Gly417Ala variant. Our results in the functional studies supported variant's potential pathogenicity in AD as indicated. The amyloid cytotoxicity and causes of presenting Parkinsonism in the patient are currently being studied in our laboratory.

Poster Presentation : LIFE.P-463

Life Chemistry

Zoom 21 FRI 16:00~17:00

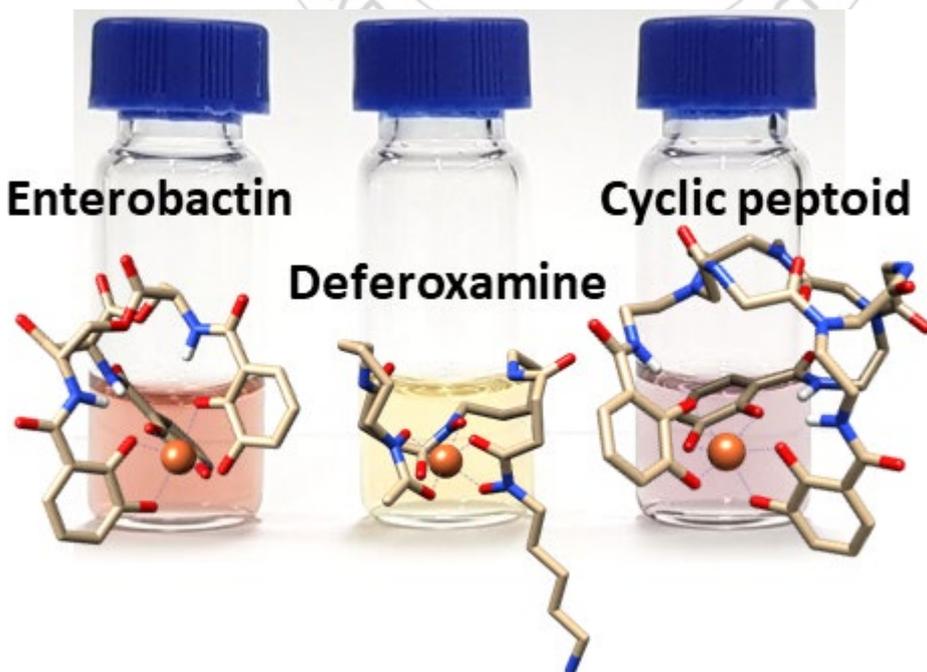
Formation of a tris(catecholato) iron(III) complex with a nature-inspired cyclic peptoid ligand

Jinyoung Oh, Sun Hee Kim¹, Jiwon Seo*

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

¹Western Seoul Center, Korea Basic Science Institute, Korea

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.¹References¹.Oh J.; Kang D.; Hong, S.; Kim, S. H.; Choi, J.-H.; Seo, J. Formation of a tris(catecholato) iron(III) complex with a nature-inspired cyclic peptoid ligand. *Dalton Trans.*, **2021**, DOI: 10.1039/D1DT00091H.



Poster Presentation : **LIFE.P-464**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Novel aromatic side chain-containing antimicrobial peptoids and their biological properties

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

¹*Gwangju Institute of Science and Technology, Korea*

Antimicrobial peptides (AMPs) are promising antibiotics against broad spectrum pathogens, including multidrug-resistant (MDR) strains and several AMPs are in clinical investigation. However, there are drawbacks such as salt sensitivity, short half-life, and low stability about proteolytic degradation which restrict their medicinal applications as an efficient versatile antibiotic. Peptoids, *N*-substituted glycine polymers, are one of the peptidomimetics. Because of their resistance against enzymatic degradations, the peptoids have been applied to antimicrobial fields to develop improved antibiotics. According to a previous biodistribution study, a peptoid appears to be too stable in the systemic circulation (>24 h), which may cause undesired toxicity. In this study, we design a peptoids library in which aromatic side chains were changed based on peptoid **1** known as an effective cationic, amphipathic, and helical antimicrobial peptoid. According to the library, we figure out the importance and tendency of some pharmacokinetic profiles of the peptoids with preserved antimicrobial activity compared to **1**. Furthermore, a mechanism study about the designed peptoids has been performed.

Poster Presentation : **LIFE.P-465**

Life Chemistry

Zoom 21 FRI 16:00~17:00

NMR Dynamics Study of target DNA recognition of Transcription Factor protein PBX4

Youyeon Go, Joon-Hwa Lee*

Department of Chemistry, Gyeongsang National University, Korea

Transcription factors (TFs) are proteins that bind specific sites or elements in regulatory regions of DNA, known as promoters or enhancers, where they control the transcription or expression of target genes. The three amino acid loop extension (TALE) homeodomain proteins are a family of transcription factor including the mammalian PBX, MEIS and PREP proteins. The PBC subclass comprises the proteins PBX1, PBX2, PBX3 and PBX4 in mammals. The TALE-HD differs from the classical HD by the insertion of three additional amino acids. These three amino acids are almost always a proline-tyrosine-proline (PYP) motif and are located between the first and second helix of the HD. The highly conserved DNA-binding TALE proteins define the family and is responsible for specific recognition of a common sequence motif. To understand the molecular mechanisms of specific DNA recognition of PBX4, we performed NMR experiments on PBX4 complexed with 10-bp DNA duplex, d(CGATGATTGA)/d(TCAATCATCG), (wt-pxDNA) and its mutants using NMR. We studied the PBX4-DNA interactions using imino proton and HSQC titrations. We also performed the ¹⁵N relaxation dispersion and imino proton exchange experiments to study the kinetics of target-specific DNA binding of PBX4.

Poster Presentation : **LIFE.P-466**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Dynamics study of transcription factor HOXA1 complexed with its target DNA using NMR

Hye Bin Ahn, Joon-Hwa Lee^{1,*}

chemistry, Gyeongsang National University, Korea

¹*Department of Chemistry, Gyeongsang National University, Korea*

In molecular biology, a transcription factor (TF) is a protein that controls the rate of transcription of genetic information from DNA to mRNA, by binding to a specific DNA sequence. Homeobox (Hox) genes encode a conserved family of transcription factor proteins that are critically important in vertebrate development. In humans, the Hox genes are distributed into four linkage groups (HOXA, HOXB, HOXC, and HOXD) comprising 39 genes located on chromosomes 7, 17, 12, and 2. Specifically, the HOXA1 may be involved in the placement of hindbrain segments in the proper location along the anterior-posterior axis during development. In this study, the backbone amide resonances of HOXA1 were assigned by multidimensional heteronuclear NMR spectroscopy. And to understand this molecular mechanism of the complex formation of HOXA1 with specific target DNA, we performed NMR experiments on HOXA1 complexed with 10-bp DNA duplex, d(5'-CGTAATGGCC-3')/d(5'-GGCCATTACG-3'), (wt-hx1DNA) and its mutants. Also we measured the HOXA1-DNA interactions using imino proton and HSQC titrations. Our study will provide DNA recognition pathway of HOXA1.

Poster Presentation : **LIFE.P-467**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Molecular structural characterization of autophagy-related protein LRRC25 from pigs

Han-ha Chai^{*}, Yunjeong Noh

Rural Development Administration, Korea

To rapidly and effectively replicate in the host, many proteins of RNA viruses have involved a range of strategies to antagonize and to evade the innate immune responses. The autophagy modulation reveals a mechanism of critical importance that allows RNA viruses to evade the host's immune system. Nonstructural protein of RNA viruses degrades the host's G3BP1 through upregulating LRRC25(leucine rich repeat-containing 25) and LRRC25 increase the genomic copies and titer of RNA viruses. In addition, other picornavirus also degrades G3BP1 by upregulating LRRC25 expression. Upon RNA virus infection, LRRC25 specifically binds to ISG15-associated RIG-I to promote interaction between RIG-I and the autophagic cargo receptor p62 and to modulate RIG-I degradation via selective autophagy. Thus, LRRC25 deficiency can enhance antiviral responses against the RNA viruses. In the study, we have investigated the relationship of conserved features between LRRC25 and compare them to those of other species. The porcine LRRC25 shares common structural and functional components with their counterparts from other species. Then we suggested insights of how key structural features of the porcine LRRC25 from model structures is associated with the central biological functions of autophagy pathways as well as a negative regulator in NF- κ B signaling pathway.

Poster Presentation : **LIFE.P-468**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Synthesis and biological evaluation of mitochondria-targeting peptoids

Jiyu Lee, Jiyoun Lee*

Global Medical Science, Sungshin University, Korea

Mitochondria-targeted delivery methods offer a straightforward approach for studying mitochondria-related diseases, and potentially streamline therapeutic development. Peptoids, poly-N-substituted glycines, are biocompatible peptidomimetics having similar physicochemical properties compared to peptides, but are proteolysis-resistant. In particular, amphipathic peptoids are membrane-permeable and their cationic charges and hydrophobicity can be readily modified for specific purposes such as cell-penetration, anti-cancer or antibacterial activity. Previously, we have identified a series of amphipathic peptoids, demonstrating efficient cell penetration and mitochondrial localization without severe toxicity. As a continued effort to find selective mitochondrial transporters, we designed new analogs with varying hydrophobicity and net charges, and investigated their mitochondrial localization and toxicity. We found that the overall increase of hydrophobicity did not affect mitochondrial localization while maintaining high cell-permeability; we also found that the positive net charge is critical for mitochondrial localization. We believe that our mitochondria-targeting peptoids provide a highly selective and robust delivery method for bioactive molecules.

Poster Presentation : **LIFE.P-469**

Life Chemistry

Zoom 21 FRI 16:00~17:00

Redesign of antimicrobial peptide to a cyclotide form to improve bioavailability

Solmin Kim

chemistry department, chonnam national university, Korea

Multi-drug resistant(MDR) emerged due to excessive use of antibiotics. To overcome this problem, the use of the antimicrobial peptides(AMPs) are being studied. One of the noticeable features of AMPs is that it is very rare for microorganisms to acquire resistance to AMPs. But the disadvantage of AMPs is that they have a low bioavailability due to their unstable forms. So in this study, AMPs were approached in the form of cyclotide. A cyclotide is a plant-derived cyclic peptide with a head to-tail cyclic backbone and three conserved disulfide bond structures. This structure confers exceptional stability against chemical, enzymatic, and thermal conditions. mBjAMP1 is an mature antimicrobial peptide from Branchiostoma japonicum that composed of 21 amino acid residues. And it contains two cysteines in the primary sequence so it can be designed as a cyclotide and adapted to be optimized. In other words, making mBjAMP1 in the form of a cyclotide is a good way to overcome the shortcomings of AMPs. First of all, A wild type sample of mBjAMP1 was made through solid-phase peptide synthesis(SPPS). And after purification using HPLC, the thiol groups in two cysteine residues were oxidized to the disulfide bond by using air as oxidant. And C(Cyclic)-mBjAMP1 was artificially created through head-to-tail cyclization of the linear peptide using a synthetic reagent, and likewise, two cysteine residues were oxidized to the disulfide bond. And after purification, the sample was finally completed. The CD spectrum was used to confirm whether c-mBjAMP1 changed its structure compared to wild type under the same conditions. And the minimal inhibitory concentration(MIC) was performed to confirm the difference of antibacterial activity.

Poster Presentation : **ORGN.P-470**

Organic Chemistry

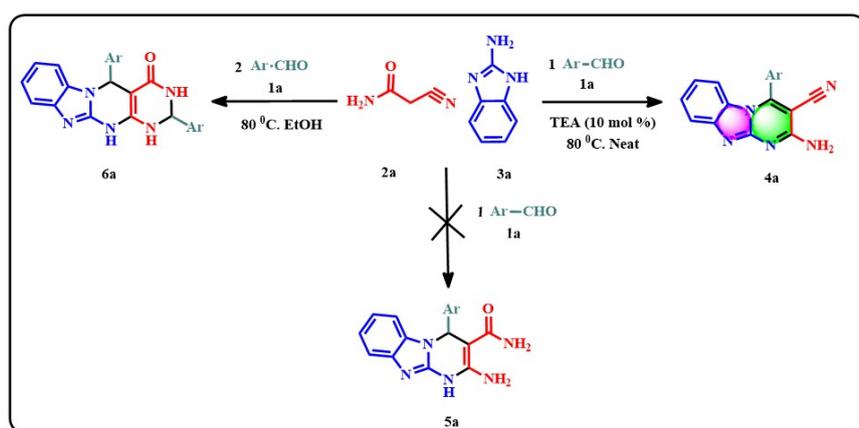
Zoom 12 FRI 15:00~16:00

Triethylamine-catalyzed unprecedented synthesis of 2- amino -4-phenylbenzo [4, 5] imidazo [1, 2-a] pyrimidine-3-carbonitrile under solvent-free condition

Maruti Yadav

Department of Display Engineering, Pukyong National University, Korea

An efficient and experimentally straightforward method for the synthesis of 2-amino-4-phenylbenzo [4,5] imidazo [1,2-a] pyrimidine-3-carbonitrile derivatives has been developed via one-pot three-component reaction of 2-Aminobenzimidazole, Cyanoacetamide and aromatic aldehydes in the presence of triethylamine under solvent-free reaction condition. This green procedure offers several advantages such as high atom economy, short reaction time, metal-free and solvent-free reaction conditions, easy work up and column chromatography-free method with a wide range of functional group tolerance. This has made the protocol sustainable and economical.



Poster Presentation : **ORGN.P-471**

Organic Chemistry

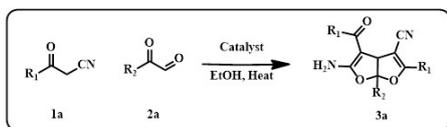
Zoom 12 FRI 15:00~16:00

Cascade Synthesis of 5-amino-4-benzoyl-2, 6a-diphenyl-3a, 6a-dihydrofuro [2, 3-b] furan-3-carbonitrile under metal-free condition

Maruti Yadav

Department of Display Engineering, Pukyong National University, Korea

A highly efficient, one-pot three-component cascade reaction for the synthesis of 5-amino-4-benzoyl-2, 6a-diphenyl-3a, 6a-dihydrofuro [2, 3-b] furan-3-carbonitrile has been discovered. The reaction sequence involves a Knoevenagel condensation of a 2-oxo-2-phenylacetaldehyde with aroylacetonitrile. Moreover, this procedure offers several advantages such as operational simplicity, good substrate, and functional group compatibility, and easily available feedstocks are the main highlights of this synthetic protocol.



Poster Presentation : **ORGN.P-472**

Organic Chemistry

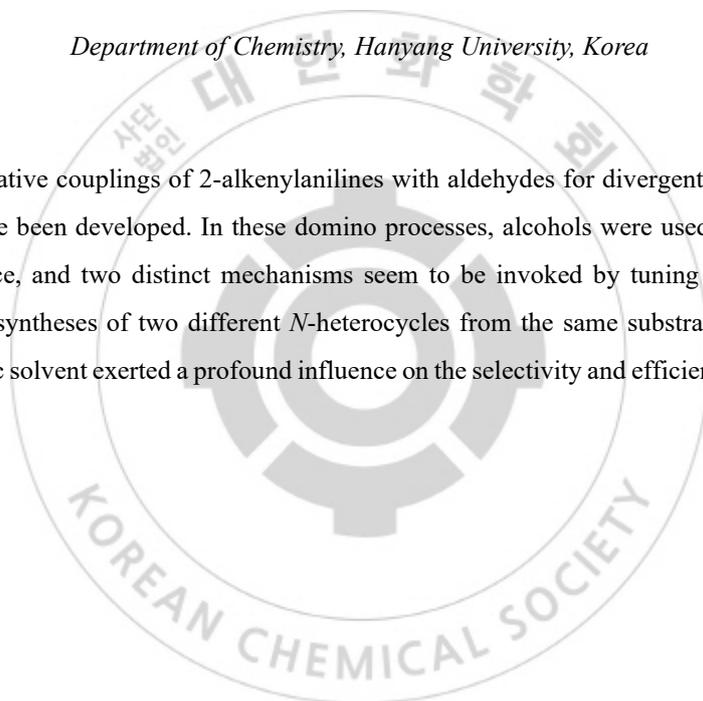
Zoom 12 FRI 15:00~16:00

Pd-Catalyzed Annulative Coupling of 2-Alkenylanilines with Aldehydes for Divergent Syntheses of Indoles and Quinolines

Youngho Kim, So Won Youn*

Department of Chemistry, Hanyang University, Korea

Pd-catalyzed annulative couplings of 2-alkenylanilines with aldehydes for divergent syntheses of indoles and quinolines have been developed. In these domino processes, alcohols were used as both solvent and the hydrogen source, and two distinct mechanisms seem to be invoked by tuning reaction parameters, enabling selective syntheses of two different *N*-heterocycles from the same substrate. The nature of the ligand and alcoholic solvent exerted a profound influence on the selectivity and efficiency in these protocols.



Poster Presentation : **ORGN.P-473**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

High-efficiency thermally activated delayed fluorescence emitters via a high horizontal dipole ratio and controlled dual emission

Youngnam Lee, Jong-in Hong*

Division of Chemistry, Seoul National University, Korea

Thermally activated delayed fluorescence (TADF) emitters containing 1,5-naphthyridine as an electron acceptor and phenoxazine and phenothiazine as electron donors, namely, 2,6-bis(4-(10*H*-phenoxazin-10-yl)phenyl)-1,5-naphthyridine (NyDPO) and 2,6-bis(4-(10*H*-phenothiazin-10-yl)phenyl)-1,5-naphthyridine (NyDPt), were developed. Because of the linear molecular structures, NyDPO and NyDPt showed high horizontal emitting dipole ratios of 81% and 84%, respectively. Furthermore, NyDPO and NyDPt exhibited TADF characteristics with photoluminescence quantum yields (PLQYs) of 79% and 45%, respectively. In particular, NyDPt showed dual photoluminescence (PL) emission from quasi-axial and quasi-equatorial conformers. However, only quasi-equatorial emission was observed in the organic light-emitting diode (OLED) at low current density, resulting in a high device efficiency despite a low PLQY. OLED devices based on NyDPO and NyDPt exhibited high external quantum efficiencies of 29.9% and 25.8%, and maximum luminance values of 33 540 cd m⁻² and 14 480 cd m⁻², respectively.

Poster Presentation : **ORGN.P-474**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Lewis acid-mediated synthesis of mono- and tris-indole adducts from chiral aziridines

Hyongjin Rhee, Hyun-Joon Ha*

Department of Chemistry, Hankuk University of Foreign Studies, Korea

Lewis acid-mediated regio- and stereoselective nucleophilic addition of 2- or 3-substituted indoles to non-activated aziridine-2-carboxaldehydes in dioxane afforded 2-(indol-3-ylhydroxymethyl)aziridines whose ring opening with various nucleophiles rendered multi-substituted tryptamine derivatives. The reaction of the same aziridine-2-carboxaldehyde with three moles of indole in dichloromethane yielded tris-indole adducts β -(3,3'-bisindolyl)methyl (BIM) tryptamines from sequential steps including nucleophilic addition to aldehyde, Michael type Friedel-Crafts alkylation of the mono-adduct followed by regio- and stereoselective ring-opening of the aziridine ring.

Poster Presentation : **ORGN.P-475**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Total Synthesis of Biemamides B and D

Nikhil Srivastava, Hyun-Joon Ha^{1,*}

Department of Chemistry, Hankuk University of Foreign Studies, India

¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

We developed an efficient linear synthetic route for the first total synthesis of 5,6-dihydrouracil containing marine natural products biemamides B and D as potential TGF- β inhibitors, from enantio-pure aziridine-2-carboxylate. Other biemamide (A, C and E) analogues, can also be synthesized by utilization of this synthetic strategy. Key features of our total synthesis includes regio- and stereoselective aziridine ring opening via azide, base-induced cyclization and sequential peptide coupling reactions. After measuring the optical properties and ECD spectra of both enantiomers, the absolute configuration of natural biemamides B and D has been revised as (-)-(5S), which is an enantiomer of the originally proposed structure (-)-(5R).

Poster Presentation : **ORGN.P-476**

Organic Chemistry

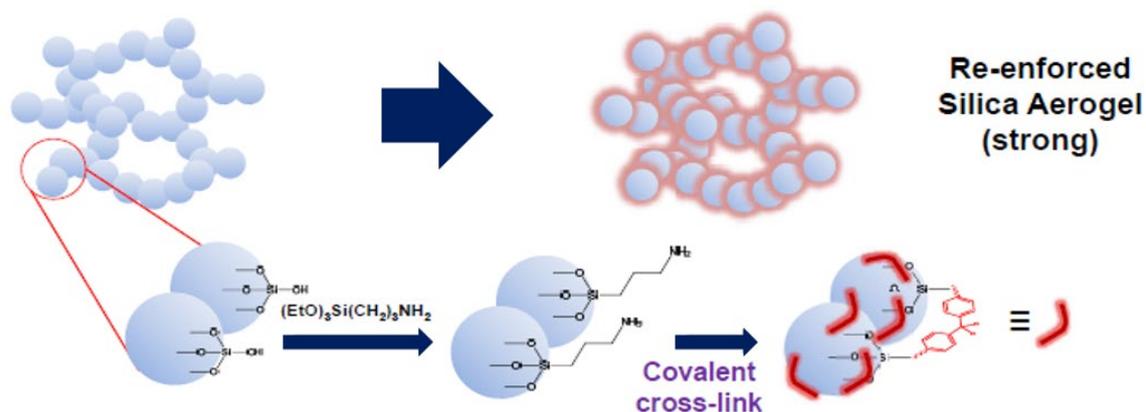
Zoom 12 FRI 15:00~16:00

Enhancing features of Silica Aerogel by cross-linking with Organic compounds

Sung Yeon Kim, Yoon Jeong Lee, Jinsung Tae*

Department of Chemistry, Yonsei University, Korea

The semiconductors of electronic devices are getting smaller every year causing a signal delay called RC delay (Resistive-capacitive delay). In order to reduce this, interlayer insulating materials with lower dielectric constant than SiO₂ has been investigated. Herein, we report organic-inorganic hybridized aerogel as a new interlayer insulating material. By hybridizing silica aerogels with organic linkers, we were able to form nano-porous thin film with high mechanical strength and low-k property. Among various synthesized linkers, aerogel with epoxy-based linker was found to be the most suitable for forming uniform nano-porous thin films.



Poster Presentation : **ORGN.P-477**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Trimethyl Lock Quinone-Functionalized Coumarin for Real-time Monitoring of NQO1 Activity in the Live Cells

Sun Young Park, Shin A Yoon, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

We developed trimethyl lock quinone-functionalized coumarin (probe **1**) as a small fluorescent probe for the imaging of NQO1 activity in the live cells. NQO1 is highly expressed in most cancer cells and it is considered as a potential biomarker of NQO1-related cancer. Probe **1** showed the high selectivity and rapid fluorescence response to the NQO1 activity. In addition, the probe is biocompatible and easily penetrates living cells. It was found that probe **1** provided relatively strong fluorescence in NQO1-positive A549 cells, unlike NQO1-negative NIH-3T3 and MDA-MB-231 cells. Therefore, we demonstrated that probe **1** can detect NQO1 activity in real time in living cells and it can also distinguish different levels of NQO1 activity in various pathological cells.

Poster Presentation : **ORGN.P-478**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Direct tracking of cell-specific activation of gemcitabine via endogenous H₂S stimulation

Shin A Yoon, Yujin Cha, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

Endogenous H₂S stimulated theranostic **H₂S-Gem** were developed for selectively ending the prognosis of cancer via activation of chemotherapeutic gemcitabine. The theranostic prodrug **H₂S-Gem** was constituted in a combination of fluorophore and gemcitabine. It showed UV-absorption at 400 nm and emission at 505 nm in the presence of exogenous H₂S. Even this theranostic **H₂S-Gem** was activated in the presence of minimal quantity (37 nM) of H₂S. The gemcitabine release process is highly selective toward H₂S, such specific activation allows gemcitabine release exclusively in cancer cells. In vitro cellular images indicated endogenous H₂S 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 H₂S formation in cancer cells. It showed selective antiproliferative activity exclusive in the cancer cells (HeLa and A549) than the human normal fibroblast cells. All of the facts advocated that it is a unique strategy for releasing cargo and selectively tracking therapeutic events to cancer cells without the support of any tumor/cancer cell-specific ligands.

Poster Presentation : **ORGN.P-479**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

A series of NAD(P)H-activable fluorescent dyes with varying intramolecular charge transfer acceptor parts

Yujin Cha, 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 components acting as a coenzyme 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 abnormal level of NAD(P)H has been found in various diseases, including cancer, neoplasia, Parkinson's and Alzheimer's diseases, etc. 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 a series of NAD(P)H-activable fluorescent probes composed of various intramolecular charge transfer (ICT) acceptor parts possessing different electron withdrawing abilities. Encountering to NAD(P)H in human cells, the probes get reduced and exhibit strong ICT emissions with different wavelengths. We expected that the probes can be applied to image living cells activating by cellular NAD(P)H.

Poster Presentation : **ORGN.P-480**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

An AIE fluorescent probe for monitoring sulfur dioxide during heat stroke

Minjoo Jung, Min Hee Lee*

Department of Chemistry, Sookmyung Women's University, Korea

We synthesized an AIEgen-based fluorescent probe capable of selectively sensing sulfur dioxide. Sulfur dioxide is known as a toxic gas or environmental pollutant. In the human system, sulfur dioxide is associated with amino acid metabolites such as cysteine. Also, sulfur dioxide exists in the human body by being divided into sulfite (SO_3^{2-}) and bisulfite (HSO_3^-). However, there are many studies showing that excessive sulfur dioxide in the human body is associated with heart disease, small intestine cancer, lung cancer, and neurological disorders. However, discrimination of the physiological functions of SO_2 in human body is restricted. Therefore, it is important to detect sulfur dioxide. AIEgens have advantages such as high quantum yield, photostability, and large Stokes shift. Because of these advantages, our probe was designed based on AIEgen. A reaction moiety capable of reacting quickly with sulfur dioxide and high selectivity was introduced, and a fluorescent probe was developed that increases the AIE effect while undergoing self-immolative cleavage and turns the ESIP effect "on". It will be able to quickly and selectively detect sulfur dioxide.

Poster Presentation : **ORGN.P-481**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Investigation of the Neuroinflammation Effects of Diosgenin Derivatives

Young Hun Yoo, Byungsun Jeon^{*}, Sanghee Lee^{*}, Jeong Tae Lee¹

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- κ B, 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. In this study, we designed and synthesized some derivatives of diosgenin by the introduction of heteroatoms at sugar linking oxygen position. Challenges in preparing the derivatives are also discussed. The prepared compounds were tested to monitor their neuroinflammatory effect and cytotoxicity. Similar results of the enantiomer of diosgenin indicate that the stereochemistry of the hydroxyl group is not critical. Enhancing the chance of hydrogen bond formation by the incorporation of amine instead of hydroxyl group appears to increase its cytotoxicity. Interestingly, dimethylamino derivative shows anti-inflammatory effect with insignificant cell toxicity ($IC_{50} = 45.1 \mu\text{M}$). Preparation of other derivatives is still on-going and their biological experiments will be followed.

Poster Presentation : **ORGN.P-482**

Organic Chemistry

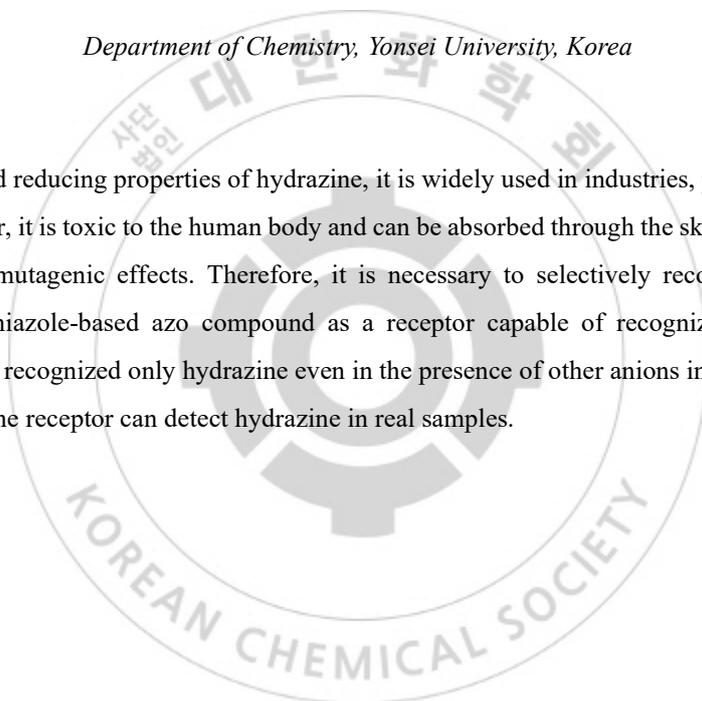
Zoom 12 FRI 15:00~16:00

A benzothiazole-based azo receptor for hydrazine detection in aqueous media

In-gyum Kim, Doo OK Jang*

Department of Chemistry, Yonsei University, Korea

Due to the basic and reducing properties of hydrazine, it is widely used in industries, pharmaceuticals, and aerospace. However, it is toxic to the human body and can be absorbed through the skin and lungs, causing neurotoxicity and mutagenic effects. Therefore, it is necessary to selectively recognize hydrazine. We designed a benzothiazole-based azo compound as a receptor capable of recognizing hydrazine. This receptor selectively recognized only hydrazine even in the presence of other anions in aqueous media. It is demonstrated that the receptor can detect hydrazine in real samples.



Poster Presentation : ORGN.P-483

Organic Chemistry

Zoom 12 FRI 15:00~16:00

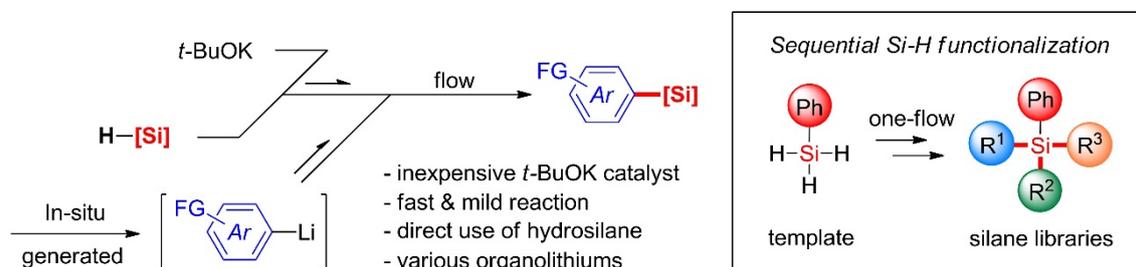
Continuous-Flow Si–H Multi-Functionalizations of Hydrosilanes Through Reaction of Aryllithiums Catalyzed by Potassium *tert*-Butoxide

Changmo Kwak, Hyune-Jea Lee, Dong Pyo Kim¹, Heejin Kim*

Department of Chemistry, Korea University, Korea

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

Synthesis of organosilicon compounds as important structural molecules has received significant attention in the various research fields including organic, material and pharmaceutical chemistry. While there are many reported studies for the formation of carbon–silicon bonds, a site-specific and atom-economic method for silylation is still highly required. Herein we present a flow approach for the silylation of organolithiums with un-functionalized hydrosilanes. Various types of in-situ generate organolithiums could be reacted with hydrosilanes in the presence of 20 mol% of potassium *tert*-butoxide (*t*-BuOK) under the mild condition within 1 minute in flow. Moreover, we successfully achieved the sequential functionalization of dihydrosilane using two different organolithiums as well. Finally, the combination of functionalizations for trihydrosilane were achieved to give every imaginable combination of tetra-substituted organosilane libraries based on a precise reaction control using an integrated one-flow system.



Poster Presentation : **ORGN.P-484**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

A pyridyl hydrazone-based chemosensor for detection of Cu^{2+} , Co^{2+} and SCN^- in aqueous solution

Jieun Park, Doo OK Jang*

Department of Chemistry, Yonsei University, Korea

Copper and cobalt ions are essential elements in the body. However, their excessive presence can cause diseases and affect environmental pollution. Therefore, it is very important to selectively recognize Cu^{2+} and Co^{2+} from the biological and environmental points of view. We designed and synthesized a pyridyl hydrazone-based chemosensor. It was expected that metal ions could be selectively detected due to the unshared electron pair of nitrogen. The chemosensor detected simultaneously Cu^{2+} and Co^{2+} ions in aqueous solution. The binding modes of sensor to Cu^{2+} and Co^{2+} were determined to be 1:1 and 2:1, respectively, through Job's plot. The resultant Cu^{2+} -complex has high selectivity for sensing SCN^- ions.

Poster Presentation : **ORGN.P-485**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

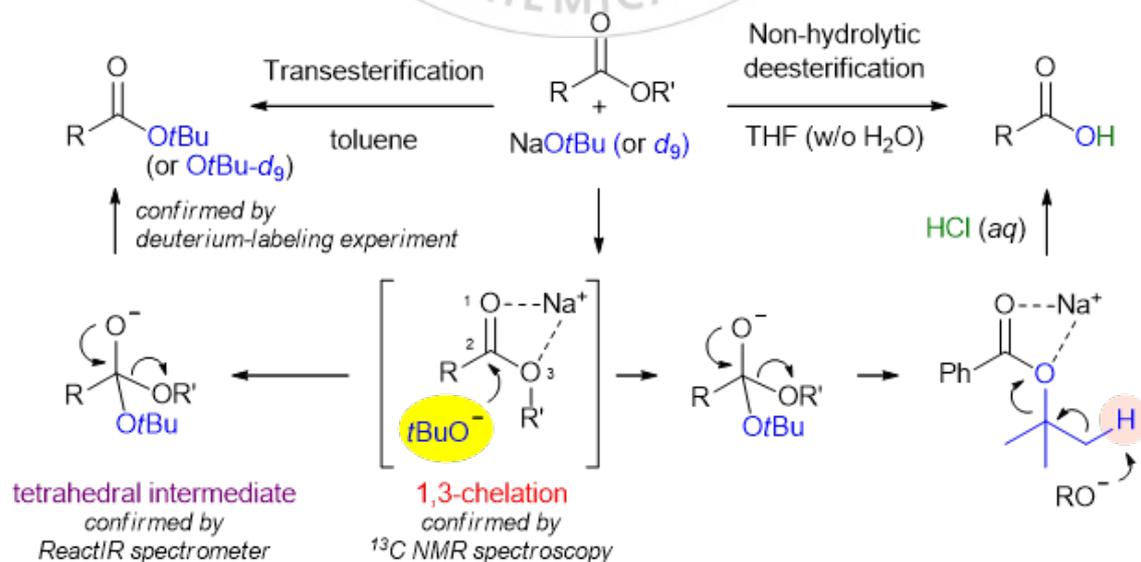
Functionalisation of esters using NaOtBu as nucleophile *via* 1,3-chelation: mechanistic investigations and synthetic applications

Hye Sung Yang, Hyun-Joon Ha^{1,*}, Jung Woon Yang^{*}

Department of Energy Science, Sungkyunkwan University, Korea

¹*Department of Chemistry, Hankuk University of Foreign Studies, Korea*

Sodium *t*-butoxide is typically considered as non-nucleophilic strong base because of steric hindrance derived from bulky alkoxide. But we developed very efficient transesterification to provide *t*-butyl ester and non-hydrolytic deesterification of esters using NaOtBu as nucleophile *via* 1,3-chelation between sodium ion and oxygen atoms in the ester. Transesterification is one of the most important reactions because it is used in various synthetic chemistry fields. We also investigated the reaction mechanism through NMR spectroscopy, React IR spectrometer, and deuterium-labeling experiment to confirm nucleophilicity of NaOtBu, the 1,3-chelation and formation of a tetrahedral intermediate. Furthermore, we successfully extended synthetic applications of the newly developed transesterification with chiral amino acid methyl esters and oxazolidin-2-ones.



Poster Presentation : **ORGN.P-486**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Improved Controllability of Fries Rearrangements Using High-Resolution 3D-Printed Metal Flow Microreaction System

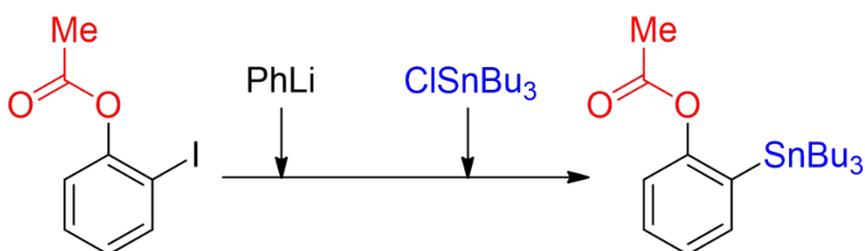
Hyune-Jea Lee, Heejin Kim, Ji Tae Kim^{1,*}, Dong Pyo Kim^{2,*}

Department of Chemistry, Korea University, Korea

¹*Department of Mechanical Engineering, The University of Hong-Kong, Hong Kong*

²*Department of Chemical Engineering, Pohang University of Science and Technology, Korea*

We fabricated the high-resolution 3D-printed stainless steel metal microreactors (3D-PMRs) with different cross-section to control ultra-fast intramolecular rearrangement reactions in a comparative manner. The 3D-PMR-C (cross section: circular channel) demonstrated the enhanced 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 precisely calculated by 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 reaction using 3D-PMR to result in high conversion and yield.

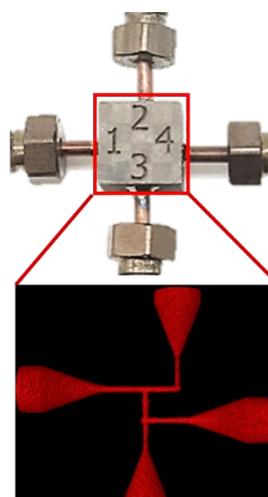


-High Resolution Metal 3D Printing

-CFD Optimization

-Precise Reaction Control

-High Mixing Efficiency



Poster Presentation : **ORGN.P-487**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Carbon Upcycling of Various C1 Sources via Iridium(NHC)-Catalyzed Transfer Hydrogenation

Yeon Joo Cheong, Hye-Young Jang^{1,*}

Department of Energy System Research, Ajou University, Korea

¹Department of Chemistry, Ajou University, Korea

Transition metal-catalyzed transfer hydrogenation (TH) of CO₂ is receiving much attention. This is because it is one of the ways to solve global warming caused by the increased CO₂ concentration. CO₂ has been used as the hydrogen acceptor in the presence of a sustainable hydrogen donor instead of H₂. Inorganic and organic carbonates derived from CO₂ have been also employed in transfer hydrogenation reactions. However, there are some challenging issues to reduced CO₂ and carbonates. Due to of the low reactivity of CO₂ and carbonates, it is important to design ligands of metal complexes. Herein, we report iridium complexes with modified *N*-heterocyclic carbene (NHC) ligand for the TH of CO₂, inorganic carbonates and organic carbonates. To increase the catalytic activity, three imidazole rings were linked by alkyl chains and reacted with iridium precursors to afford mono-and binuclear complexes. The detailed results will be discussed.

Poster Presentation : **ORGN.P-488**

Organic Chemistry

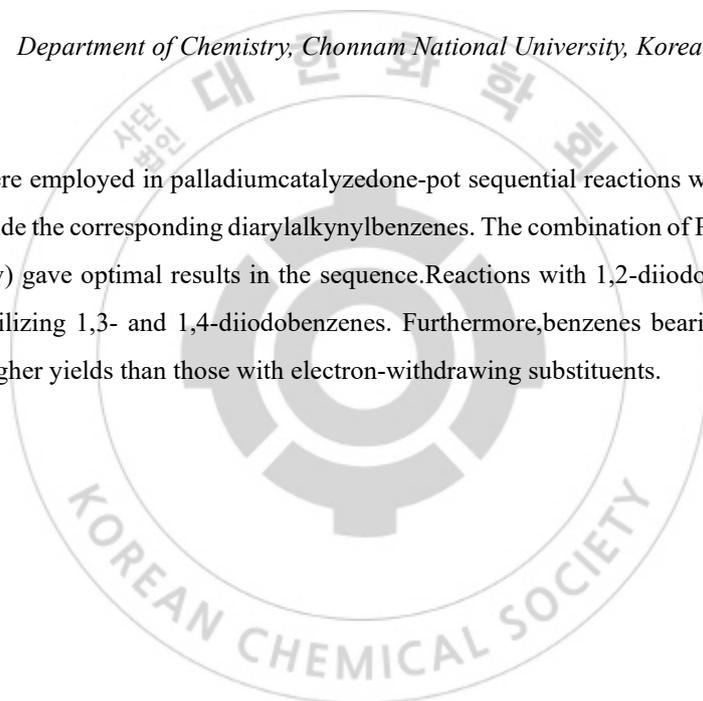
Zoom 12 FRI 15:00~16:00

Diiodobenzenes, Propiolic Acid, and Aryl Halides for the Synthesis of Diarylalkynyl Arenes Sequential One-Pot Coupling Reactions

An Seunghwan, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Diiodobenzenes were employed in palladiumcatalyzedone-pot sequential reactions with propiolic acidand aryl halides to provide the corresponding diarylalkynylbenzenes. The combination of Pd(PPh₃)₄ (10 mol%) andDBU (5.0 equiv) gave optimal results in the sequence.Reactions with 1,2-diiodobenzene gave higher yields thanthose utilizing 1,3- and 1,4-diiodobenzenes. Furthermore,benzenes bearing electron-donating substituents gavehigher yields than those with electron-withdrawing substituents.



Poster Presentation : **ORGN.P-489**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Flow-assisted Synthesis of [6,4]CPPy in Eco-Friendly Solvent through Serial Microreactions

Yongju Jeon, Hyune-Jea Lee¹, Heejin Kim^{1,*}

Department of chemistry, Korea University, Korea

¹*Department of Chemistry, Korea University, Korea*

The development of 2,2'-bipyridine embedded CPP(CPPy) ligand with tunable electronic structures and unique three-dimensional molecular shapes has provided access to an abundance of metal coordination complexes for a wide range of applications. However, the reported synthetic routes for CPPy required time- and cost-consuming multi-step conditions which stands as a main hurdle for wide applications of the CPPy. Herein, we report atom-economical and environmentally friendly synthesis of cyclo[6]paraphenylene[4]2,5-pyridylidene([6,4]CPPy) by using flow microreactors with 2-methyltetrahydrofuran (2-Me THF) which is known as more eco-friendly solvent than tetrahydrofuran. We proved that halogen-lithium exchange reaction as well as nucleophilic addition of organometal reagent was successfully conducted even in 2-Me THF. Furthermore, a selective nucleophilic addition of unprotected 1,4-benzoquinone and continuous alcohol protection successfully provided L-shaped precursor in high yield using the microfluidic device. The obtained L-shaped product was converted into an U-shaped precursor, important building block, for the synthesis of [6,4]CPPy. Finally, we calculated absorption and fluorescence properties of [6,4]CPPy, which demonstrated its potential of luminescent materials and the ligand for the organometallic complexes.

Poster Presentation : **ORGN.P-490**

Organic Chemistry

Zoom 12 FRI 15:00~16:00

Formation of stable PDA liposome and application to paper sensor using flow chemistry

Galam Jung, Kiok Kwon*

Korea Institute of Industrial Technology, Korea

PDA, one of the conjugated polymers that causes color shift under the influence of external stimuli, has been used as a colorimetric sensor. PDA is self-assembled into liposomes having a circular lipid bilayer structure in an aqueous solution. Preparation of mono-disperse PDA liposome particle with long term stability is a crucial challenge to be used as to be utilized as a superior sensor material. In this study, a new method for preparation of stable liposome particle by using flow chemistry was proposed. In a conventional method for forming liposomes, batch method, it is difficult to fine-tune the major physical factors in liposome formation. We settle down this issue by utilizing a flow chemistry in liposome formation process. Precise control of flow rate and physical condition Inside microfluidic channels permit the successful formation of stable, mono-disperse liposome particle. The size of liposome particle prepared and storage stability in an aqueous solution over time were confirmed using PSA (particle size analyzer), and the characteristics of photopolymerization and temperature detection were confirmed by UV-Vis spectra. Compared with the batch reaction, this study showed the superiority of the stability (particle size, monodispersity, storage stability) of PDA liposomes formed by flow chemistry. This will enable liposomes formed with a new strategy to be applied as sensors in various fields.

Poster Presentation : **ORGN.P-491**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

Preparation of covalent organic framework using naphthorosarin(3Bpin)

Yebin Park, Chang Hee Lee^{1,*}, Woo-Dong Jang^{2,*}

Department of chemistry, Yonsei University, Korea

¹*Department of Chemistry & Biochemistry, Kangwon National University, Korea*

²*Department of Chemistry, Yonsei University, Korea*

Covalent organic frameworks (COFs) are crystalline porous materials connected through covalent bond and they have paid attention to potential of various application with other organic frameworks like metal organic frameworks (MOFs) and hydrogen bonded organic frameworks (HOFs). COFs have specific advantages compare with other organic frameworks, such as high thermal stabilities and low mass densities. COFs can be prepared by solvothermal synthesis through the formation of boronate bond as a typical covalent bond. Naphthorosarin is a type of expanded porphyrin that has β and β' conjugation of pyrrole. Although rosarin has non-aromatic character because it has distorted, the naphthorosarin has antiaromatic character with 24 π -electrons system owing to the planar structure. In this study, I have synthesized naphthorosarin(3Bpin) and COFs that boronated naphthorosarin was reacted with catechol of 1,2,4,5-tetrahydroxy benzene through boronate bond and these materials has been a new porous 2D network structure. The naphthorosarin COFs was crystalized by solvothermal method and characterized by scanning electron microscope (SEM). Because naphthorosarin is typical antiaromatic structure, we can expect to find new functions of rosarin-based COF.

Poster Presentation : **ORGN.P-492**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

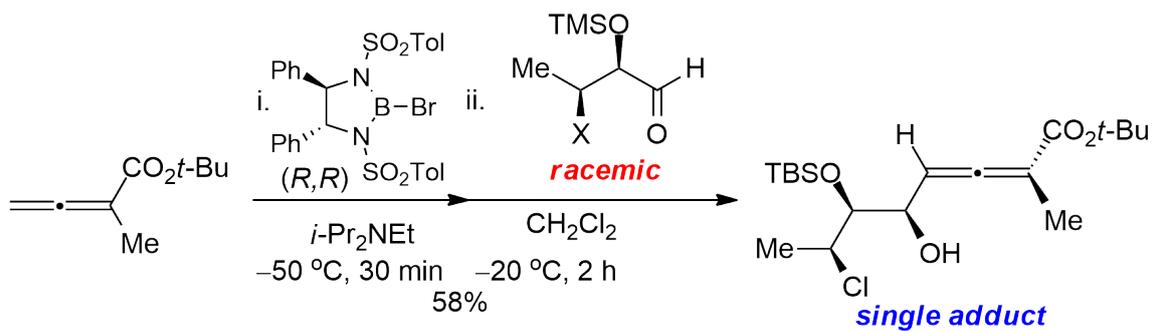
Optimal Kinetic Resolution of Racemic Aldehydes through Asymmetric Allenoate Gamma Addition: Correction of All Xylogibactone Family

Zhang Aimin, Euijin Park¹, Sehui Yang¹, Jimin Kim^{1,*}

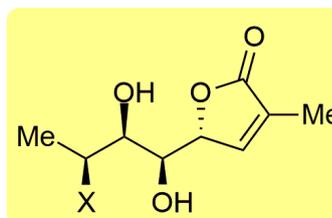
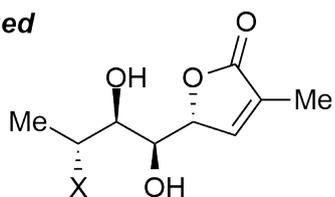
Department of Chemistry, Chonnam National University, China

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

The elegant simplicity with which nature assembles complex molecular frameworks is breathtaking. Among a variety of synthetic methods for the synthetic routes of natural gamma-lactone polyketide (+)-xylogibactone A, B, and C have been explored in four-step sequence for the first time. This highly stereoselective synthesis of (+)-xylogibactones involves three major key transformations: i) highly stereoselective allenoate gamma-addition of racemic aldehydes through an optimal kinetic resolution to provide only single adduct. ii) regiospecific cyclization of gamma-adducts through gold catalysis to provide gamma-lactone unit. This investigation led to the correction and verification of the known relative and absolute stereochemistry.

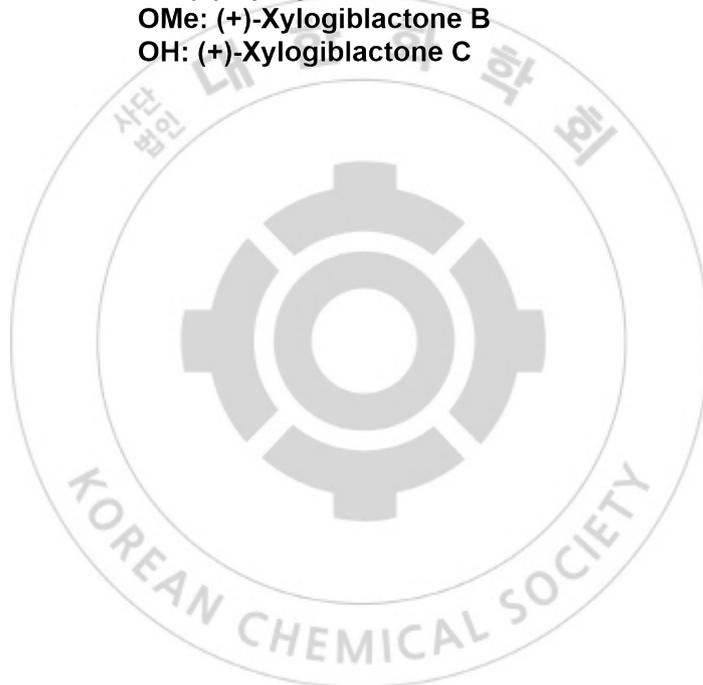


Reported



Corrected

X = Cl: (+)-Xylogibactone A
 OMe: (+)-Xylogibactone B
 OH: (+)-Xylogibactone C



Poster Presentation : **ORGN.P-493**

Organic Chemistry

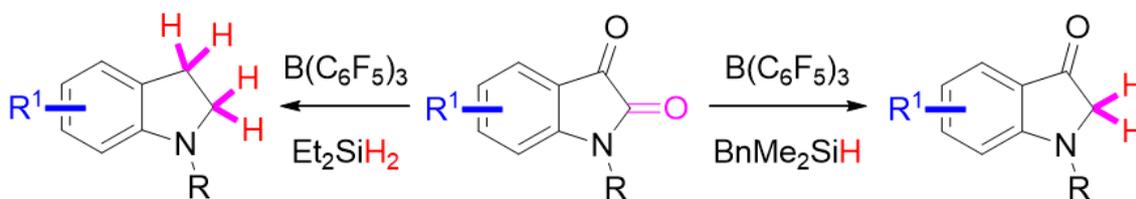
Zoom 12 FRI 16:00~17:00

B(C₆F₅)₃-Catalyzed Highly Chemoselective Reduction of Isatins: Synthesis of Indolin-3-ones and Indolines

Jaehwan Kim, Haye Min Ko*

Department of Bio-nanochemistry, Wonkwang University, Korea

A chemo- and site-selective reduction reaction of isatin derivatives using catalyst B(C₆F₅)₃ and hydrosilanes is described. This transformation is operationally simple, proceeds under mild conditions, and is resistant to various functional groups. Thus, this efficient reaction using a combination of B(C₆F₅)₃ and BnMe₂SiH or B(C₆F₅)₃ and Et₂SiH₂ could potentially be utilized to produce various indolin-3-ones and indolines, without the need for multistep procedures and metal catalysis conditions.



- **Nonmetal catalysis, mild conditions**
- **Rapid access to indolin-3-ones and indolines**
- **Highly chemo- and site-selective synthesis**

Poster Presentation : **ORGN.P-494**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

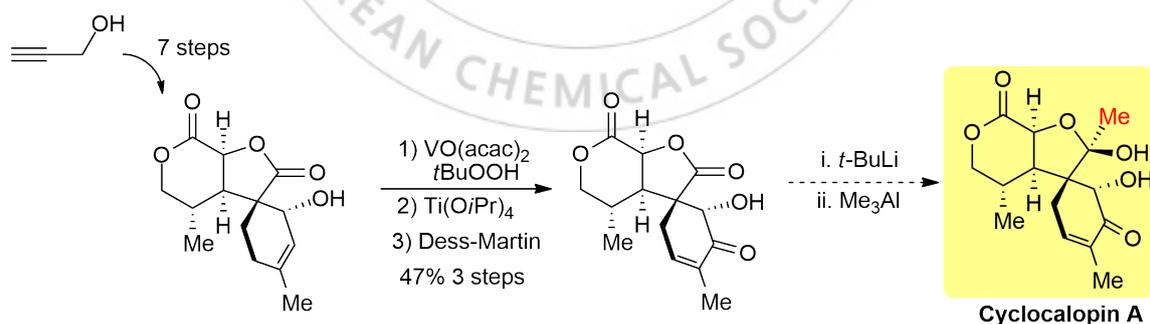
Elaboration of Spiro-unit for the Construction of Functional Framework in Cyclocalopin A

Zhang Aimin, Hyeonjong Choi¹, Jimin Kim^{1,*}

Department of Chemistry, Chonnam National University, China

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

The elegant simplicity with which nature assembles complex molecular frameworks is breathtaking. Recently, we have developed reaction routes from allenyl glyoxylate to tricyclic skeleton of cyclocalopin natural products in 7 step sequence from readily available propargyl alcohol. Efficient construction of the spiro-system through three steps chemical conversions described below. We would like to present herein several crucial points that have emerged during our recent investigations for the synthesis of naturally occurring cyclocalopin series: i. stereoselective elaboration of a spiro-system in cyclocalopin structure. ii. Chemical conversions through functional group transformations. iii. Toward a synthesis of cyclocalopin A.



Poster Presentation : **ORGN.P-495**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

Synthesis and characterization of novel Heteroleptic Iridium(III) Complexes with bulky ligands for Solution-Processed Organic Light-Emitting Diodes

Seoil Kim, Do-Hoon Hwang*

Department of Chemistry, Pusan National University, Korea

We synthesized and characterized the new orange-emitting iridium(III) complexes, (DMBT)2Ir(acac) and (TBT)2Ir(acac), based on either 2-(3,4-dimethylphenyl)benzo[d]thiazole (DMBT) or 2-(4-(trimethylsilyl)phenyl)benzo[d]thiazole (TBT) as the cyclometalated main ligands and acetylacetonate (acac) as an ancillary for solution-processed organic light-emitting diodes (OLEDs). The iridium(III) complex, (BT)2Ir(acac), which consists of 2-phenylbenzo[d]thiazole (BT) as the main ligand and acac as the ancillary ligand, was also synthesized as a reference. The electrochemical, photophysical, and electroluminescent (EL) properties of these iridium(III) complexes were studied. The OLED fabricated using (TBT)2Ir(acac) showed a significantly improved luminance and external quantum efficiency (EQE) with prevented concentration self-quenching at high doping concentrations by introducing big trimethylsilyl groups. The EL spectrum of (TBT)2Ir(acac) exhibited an emission maximum at 578 nm with a FWHM of 74 nm and Commission Internationale de L'Eclairage coordinates of (0.55, 0.44) at 1000 cd/m². The device with 7 wt% (TBT)2Ir(acac) doping concentration exhibited a maximum luminance of 6,837 cd/m², maximum luminous efficiency of 25.26 cd/A, power efficiency of 12.37 lm/W, and EQE of 9.94%.

Poster Presentation : **ORGN.P-496**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

Efficient organic catalyst for hydrogenation of Benzoxazines

Sungmin Kang, Taek Hyeon Kim*

School of Chemical Engineering, Chonnam National University, Korea

This study reports on the isothiuronium 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 isothiuronium iodide as the catalyst. Various 3,4-dihydro-2H-1,4-benzoxazines were obtained in high yield in a short reaction time under mild room temperature conditions.

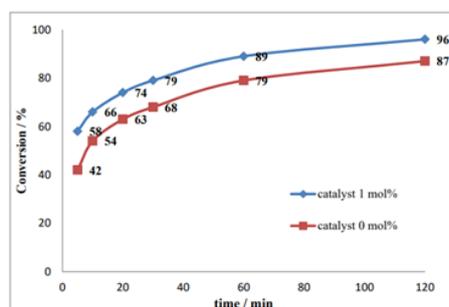
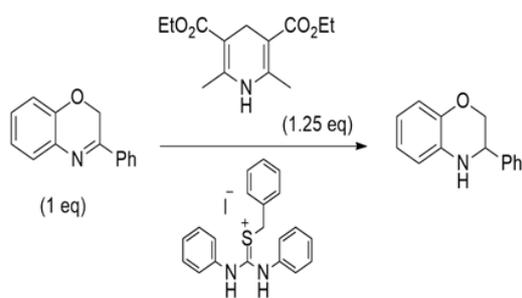


Figure 1. Formation of 3-phenyl-3,4-dihydro-2H-1,4-benzoxazine with time transition hydrogenation of 3-phenyl-2H-1,4-benzoxazine with Hantzsch ester in the presence of S-benzyl-N,N'-diphenyl isothiuronium iodide.

Poster Presentation : **ORGN.P-497**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

DMSO-Promoted α -Hydrolysis of α -Halohydroxamates under Mild conditions

ChangYoon Lee, Sung-Gon Kim*

Department of Chemistry, Kyonggi University, Korea

α -Hydroxy carbonyl compounds, including α -hydroxy ketones amides, are important structural motifs that are present in many biologically active and pharmaceutically relevant compounds like cefamandole, paeonilactone B, LY-411575 . Therefore, the development of methods for synthesizing α -hydroxy carbonyl compounds have been investigated in recent years. We also have been studied for nucleophilic α -hydrolysis of α -halohydroxamates via azaoxyallyl cation intermediate. in order to progress the mild strategy for the synthesis of α -hydroxy carbonyl compounds, dimethyl sulfoxide (DMSO) was used a catalyst, while water served as the nucleophile. This method was successfully applied to α -halo- α -arylhydroxamates, α -halo- α -alkylhydroxamates, and α -halo- α -dialkylhydroxamates. Furthermore, the α -hydroxylation of α -halo- α -dialkylhydroxamates with water was also achieved without DMSO catalysis.

Poster Presentation : **ORGN.P-498**

Organic Chemistry

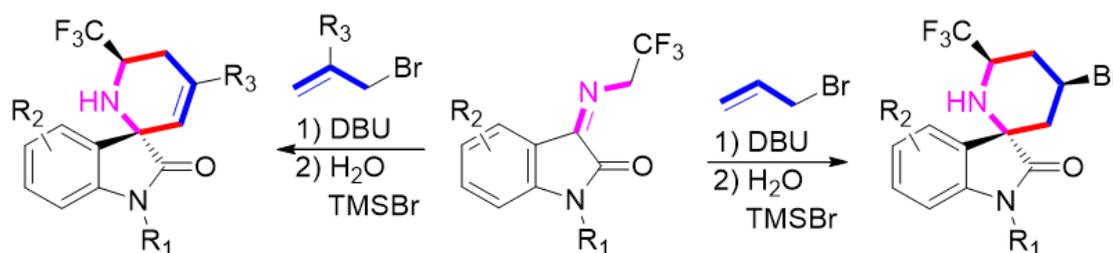
Zoom 12 FRI 16:00~17:00

Synthesis of Six-Membered Spiro Azacyclic Oxindole Derivatives *via* a One-Pot Process of Umpolung Allylation/Aza-Prins Cyclization

Se Yeon Park, Haye Min Ko*

Department of Bio-nanochemistry, Wonkwang University, Korea

An unprecedented synthetic approach involving umpolung allylation/aza-Prins cyclization of *N*-2,2,2-trifluoroethylisatin ketimines is described. The reactions proceed smoothly with allyl bromide in the presence of 1,8-diazabicyclo[5.4.0]undec-7-ene, H₂O, and trimethylsilyl bromide; this one-pot protocol allows access to six-membered spiro azacyclic oxindole derivatives in good to excellent yields. Notably, while the general aza-Prins cyclization involves amines and aldehydes, the present synthetic strategy represents the first aza-Prins cyclization that utilizes the umpolung property of *N*-2,2,2-trifluoroethylisatin ketimines.



- **One-pot process, mild conditions, short reaction times**
- **Rapid access to spiro[indoline-3,2'-piperidin]-2-ones and 5',6'-dihydro-1'H-spiro[indoline-3,2'-pyridin]-2-ones**

Poster Presentation : **ORGN.P-499**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

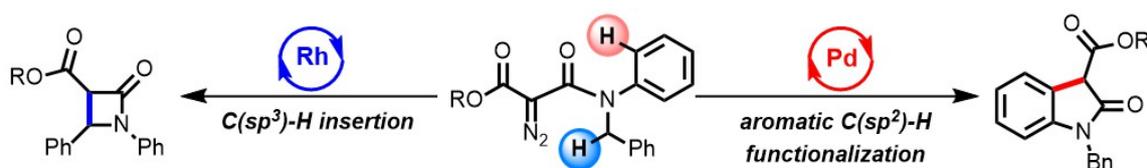
Catalyst-Controlled Divergent C(sp³)-H/C(sp²)-H Bond Functionalizations of α -Diazoamides

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

Chemistry and Nanoscience, Ewha Womans University, Korea

Transition metal-catalyzed C-C bond formation via C-H bond functionalizations has emerged as an indispensable tool in organic synthesis. Particularly, intramolecular insertion of metal carbenoids into C-H bonds has become one of the most powerful strategies to synthesize the heterocycles.¹ Despite significant improvements, site-selective C-H bond functionalization is still challenging due to the requirement of controlling the distinctive steric and electronic properties.² Herein, we present an unprecedented example of catalyst-controlled divergent C(sp³)-H/C(sp²)-H bond functionalizations with α -diazoamides.³ It was observed that the rhodium catalyst undergoes C(sp³)-H bond insertion to afford β -lactam derivatives, whereas the palladium catalyst undergoes electrophilic aromatic C(sp²)-H bond functionalization affording indolin-2-one derivatives. Moreover, it was found that the ester group of α -diazoamides plays a critical role in giving such site selectivity between C(sp³)-H and C(sp²)-H bonds.

1.(a) Borpatra, P. J.; Deka, B.; Deb, M. L.; Baruah, P. K. *Org. Chem. Front.* **2019**, *6*, 3445. (b) Sole, D.; Amenta, A.; Mariani, F.; Bennasar, M.-L.; Fernandez, I. *Adv. Synth. Catal.* **2017**, *359*, 3654. (c) Lombard, F. J.; Coster, M. J. *Org. Biomol. Chem.* **2015**, *13*, 6419.2.(a) Ping, L.; Chung, D.S.; Bouffard, J.; Lee, S.-g. *Chem. Soc. Rev.* **2017**, *46*, 4299. (b) Davies, H. M. L.; Mortana, D. *Chem. Soc. Rev.* **2011**, *40*, 1857.3.Lee, Y. L.; Choi, K. I.; Lee, S.-g. **2021**, manuscript in preparation.



Poster Presentation : **ORGN.P-500**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

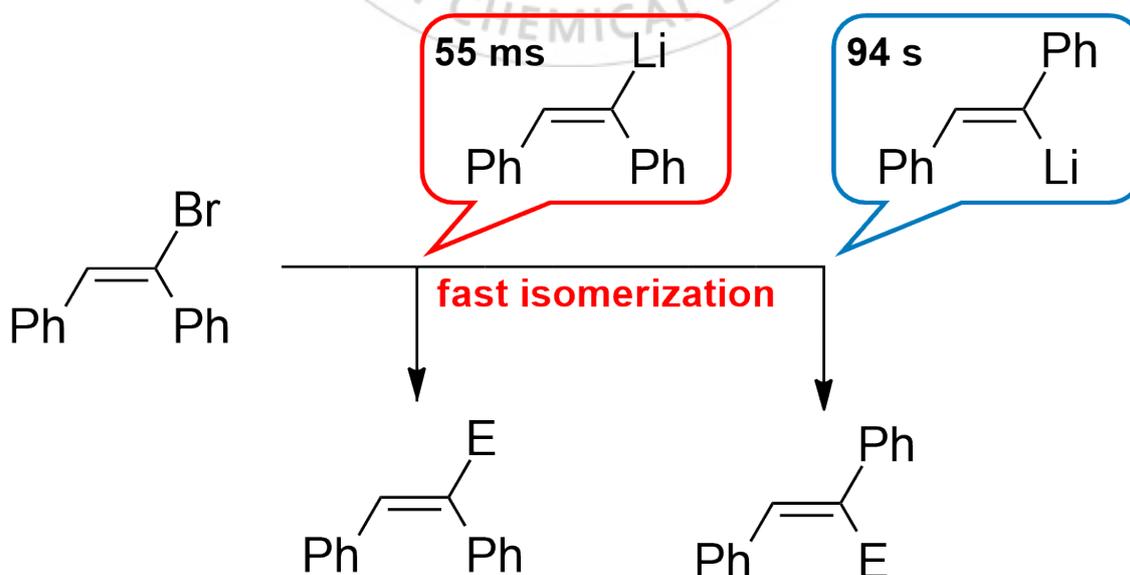
Control of rapid isomerization of *cis-trans* α -anionic stilbene in flow microreactors and application to synthesize regioselective α -functionalized stilbenes

Nayoung Kim, Hyune-Jea Lee¹, Heejin Kim^{1,*}

Chemistry, Korea University, Korea

¹Department of Chemistry, Korea University, Korea

Stilbene has difficulty in regioselective synthesis due to rapid *cis-trans* isomerization of α -anionic stilbene. However, the use of flow microreactors enabled the synthesis of highly regioselective α -anionic stilbene through precise control of reaction time by milliseconds to seconds scale. The generated *cis*- and *trans*- α -anionic stilbenes were subsequently reacted with various electrophiles in integrated flow microreactors. Especially, *cis*-stilbenyl borate was successfully synthesized and utilized in versatile synthetic applications. Furthermore, our well-established flow systems enable to synthesize precursors of (*E*)- and (*Z*)-tamoxifen, commercially available drug compound, with high regioselectivity and productivity.



Poster Presentation : **ORGN.P-501**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

Effect of Ir(NHC)-Bimetallic Structure in Guerbet Reaction : Catalytic Activity and Reaction Rate.

Mi-hyun Lee, Hye-Young Jang^{1,*}

Department of Energy System Research, Ajou University, Korea

¹Department of Chemistry, Ajou University, Korea

Transition metal-catalyzed cross-coupling via the borrowing hydrogen strategy can be used for the synthesis of high molecular weight branched alcohols which can be applied to detergents and lubricants. Alcohols are not regarded as favorable electrophiles. However, transition metal catalysts make alcohols undergo electrophilic reactions via borrowing hydrogen strategy. Using this strategy, we conducted dimerization of primary alcohols (Guerbet reaction). Furthermore, we suggest a plausible mechanism utilizing kinetic studies and the low mass analysis to probe intermediates. Herein, we demonstrate the unique effect of the bimetallic structure of catalysts on the yield and the rate of Guerbet reaction. Our efficient catalysts are effective for the various primary alcohol reactions to afford industrially important high molecular weight alcohols.

Poster Presentation : **ORGN.P-502**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

An aza-BODIPY based fluorescent probe containing colorimetric change for detection of cysteine

Seongman Lee, Thanh Chung Pham, Chaeon Bae, Sumin Jeon, Songyi Lee^{1,*}

Department Interdisciplinary Program of Biomedical, Mechanical and Electrical Engineering, Pukyong National University, Korea

¹*Department of Chemistry, Pukyong National University, Korea*

Intracellular thiols, such as cysteine (Cys), homocysteine (Hcy) and glutathione (GSH), play a crucial role in cellular growth, metabolism, maintaining biological systems. However, abnormal concentrations of thiols are implicated in a variety of health conditions, such as liver damage, skin lesions, delayed growth and edema. Therefore, it is highly important to report changes in thiol concentrations via monitoring. A fluorescent probe (BDP-1), which is based on aza-BODIPY, was developed for detection cysteine (Cys). BDP-1 showed the red-shift of fluorescence to BDP-OH by sulfonyl group combines with Cys. Redshift of absorption wavelength has a similar tendency to result of time-dependent DFT (TD-DFT) calculation. Detection limit of Cys was calculated as 3.64 μM in PBS (pH 7.4)/THF (5/5). We confirmed potential as not only fluorescence sensor, but also colorimetric sensor.

Poster Presentation : **ORGN.P-503**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

Optical and Electrochemical properties of Bis-Quinoxaline-TTF Sulfoxide Derivatives.

Ji Yoon Lee, Jung Su Park^{1,*}

department of chemistry, Sookmyung women's university, Korea

¹*Department of Chemistry, Sookmyung Women's University, Korea*

Abstracts, We present the synthesis, characterization, and properties of sulfoxide derivatives of the symmetrically fused quinoxaline TTF derivatives **1**, prepared from the m-CPBA oxidation reaction. The stoichiometric reactions between the compound **1** and m-CPBA produces the corresponding mono-sulfoxide(-S=O) (**2**) and tri-sulfoxide (**3**) derivations, respectively (Figure 1a). The oxidation on **1** result in the drastic decrease in its electron-donating ability, as reflected in their first oxidation potential. The optical absorption (Figure 1b) and emission (Figure 1c) band of sulfoxides (**2-3**) were greatly shifted to shorter wavelength region, but different by degrees of oxidation, compared to compound **1**. As it can be seen from Figure 1d, Bis-Quinoxaline-TTF mono-sulfoxide (**2**) also exhibited solvent-polarity-dependent solvatochromism. In comparison to the parent Bis-quinoxaline-TTF, optical and electrochemical properties of its sulfoxide forms as well as their protonation forms will be discussed in terms of UV-Vis, fluorescence, NMR, and cyclic voltammograms.

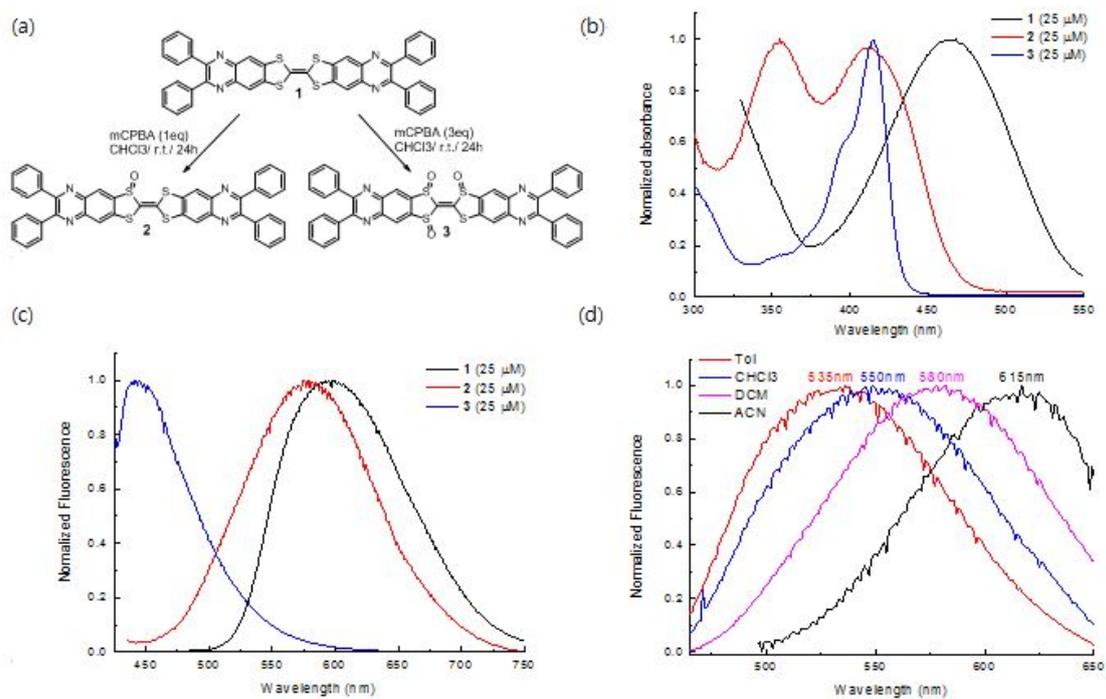


Figure 1. (a) Synthetic scheme, (b) normalized UV-Vis spectra and (c) normalized Emission spectra of the quinoxaline fused TTF sulfoxide derivatives **1-3**, and (d) normalized Emission spectra of **2** in different solvents.



Poster Presentation : **ORGN.P-504**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

A Heavy-Atom-Free Photosensitizer for Sustainable Photodynamic Therapy Using 2-Pyridone Moiety.

Yeonghwan Choi, Songyi Lee^{1,*}

Department Interdisciplinary Program of Biomedical, Mechanical and Electrical Engineering, Pukyong National University, Korea

¹*Department of Chemistry, Pukyong National University, Korea*

Photodynamic therapy (PDT) is one of the ways to treat cancer using photosensitizer (PS) and light. However, PDT has a limitation in that its effect is lowered because the oxygen concentration in cancer cells is low. To overcome this problem, it has been reported that both oxygen atoms of naphthalimide is replaced with sulfur can generate reactive oxygen species (ROS) via both type-I and type-II mechanisms. Furthermore, a 2-pyridone moiety was used to continuously release singlet oxygen even in the dark. Singlet oxygen generated by PS reacts with 2-Pyridone to form endoperoxide, and the endoperoxides of 2-pyridone returns to its original form by releasing singlet oxygen through a thermal cycloreversion process. As a result, PDT can occur continuously in both light cycles and in the dark.

Poster Presentation : **ORGN.P-505**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

Enantioselective Michael addition, DFT calculations and reaction mechanism studies using chiral (*R,R*)-1,2-diphenylethylenediamine derived thioureas

Byung Kook Ahn, Jae Ho Shim*

Department of Chemistry, Korea University, Korea

The Michael addition is valuable and still used very widely. Because It is cost-effective and does not leave metal waste that can cause environmental pollution with organocatalyst. Derived thiourea catalyst was developed and used to asymmetric Michael additions of aromatic ketones, β -ketoester, and dialkyl malonate to trans- β -nitroalkene compounds. In addition, isopropyl or trifluoromethyl-substituted thiourea catalysts were developed and applied to asymmetric Michael additions of nitroalkenes. Further we studied reaction mechanisms by comparing ΔG of transition states with DFT calculations. Moreover it enables gram-scale synthesis for drug synthesis and recycling of the catalysts. Finally the catalysts demonstrated high chemical yields and enantioselectivities under neutral conditions.

Poster Presentation : **ORGN.P-506**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

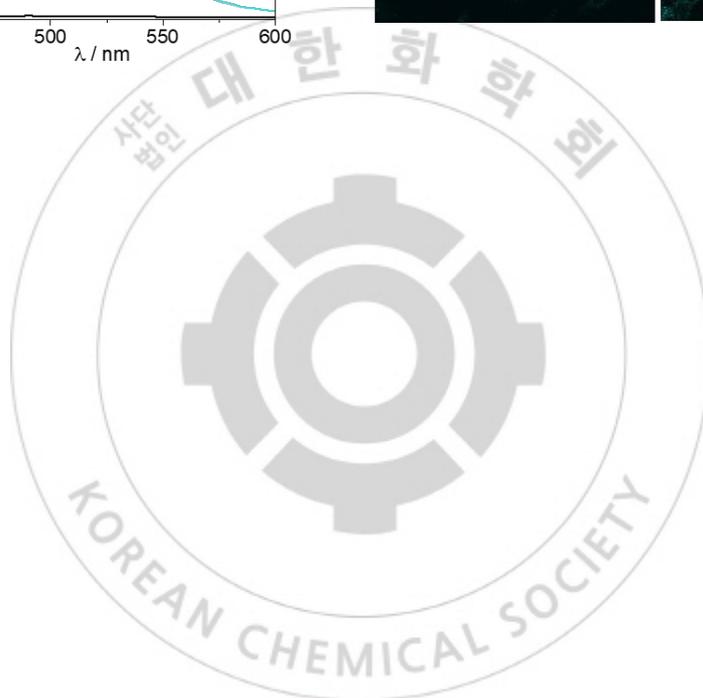
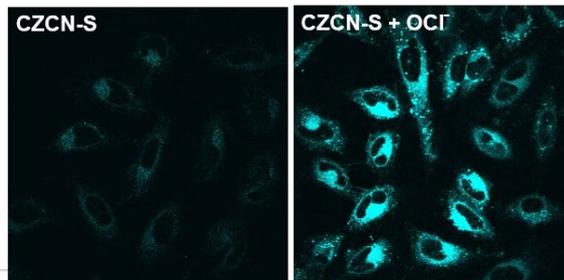
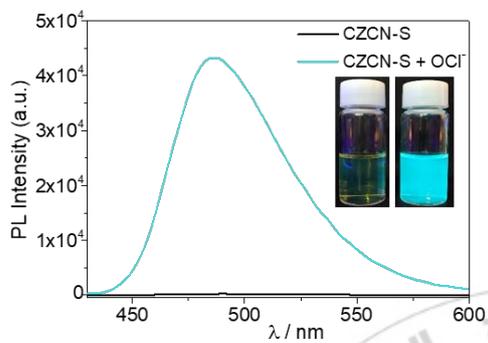
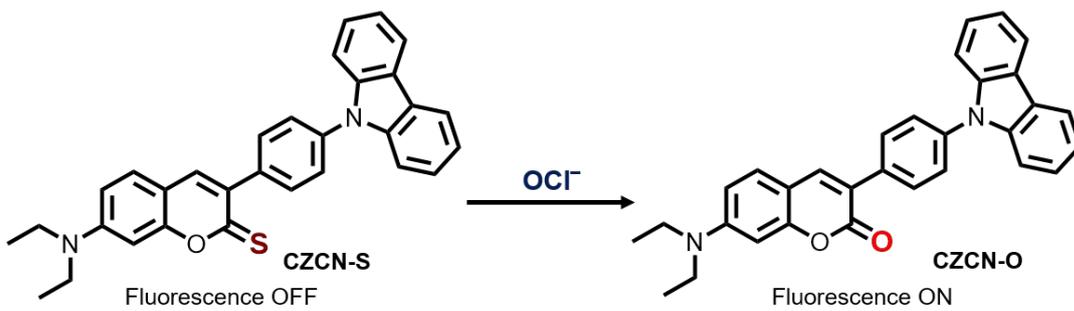
Design and synthesis of thiocoumarin-based turn-on fluorescent probe for hypochlorite detection

Jeongsun Ha, Sunnam Park^{1,*}, Juyoung Yoon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

¹*Department of Chemistry, Korea University, Korea*

The development of effective fluorescent probes for the detection of ClO⁻ is highly desired for diagnosing ClO⁻-related diseases, as well as environmental safety. Although thiocoumarin derivatives have been successfully utilized as turn-on fluorescent probes for the detection of ClO⁻, these probes still could not detect ClO⁻ selectively. In this work, a novel thiocoumarin-based turn-on fluorescence probe for the detection of ClO⁻ was designed. The addition of ClO⁻ to the PBS buffer (pH = 7.4, containing 50% acetonitrile) of CZCN-S resulted in a remarkable fluorescence enhancement with an emission maximum at 486 nm, indicating the sensitive OFF-ON fluorescence sensing of ClO⁻. The detection limit for the detection of ClO⁻ in 50% aqueous acetonitrile was calculated to be 0.17 μM. The investigation of sensing behavior toward various analytes revealed that the probe CZCN-S had an excellent selectivity for ClO⁻. The recognition mechanism was attributed to the ClO⁻-induced conversion of thiocarbonyl coumarin into its oxo analogue through oxidative desulfurization. Moreover, in vitro cell studies demonstrated that CZCN-S could be used as an effective fluorescent probe for the detection of ClO⁻ in living cells.



Poster Presentation : **ORGN.P-507**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

Selective Electrooxidation Reaction of Sulfide under Constant Current Conditions

Jin Kyu Park, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

Many synthetic methods are known to oxidize sulfide to sulfoxide and sulfone using an oxidizing agent. However, we developed a synthetic method that selectively anode oxidize sulfide into sulfoxide and sulfone at room temperature without an oxidizing agent using electrochemical reaction under constant current conditions. Also, we can say that it is more environmentally friendly by using green solvent. The selectivity of the oxygenation products (sulfoxides vs. sulfones) can be switched by simply changing the charge under constant current conditions. Various aromatic and alkyl sulfides can be transformed directly into the corresponding sulfoxides or sulfones with high yield and selectivity. Through a control experiment, we found that the oxygen source of the oxidized product came from water.

Poster Presentation : **ORGN.P-508**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

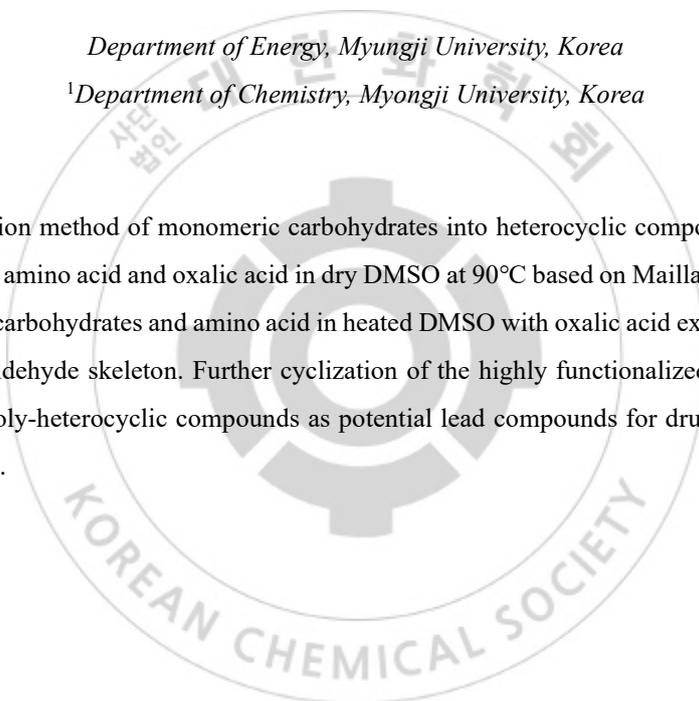
One-Pot Conversion of Carbohydrates into Pyrrole-2-carbaldehydes as Sustainable Platform Chemicals

Lina Gu, Sangho Koo^{1,*}

Department of Energy, Myungji University, Korea

¹*Department of Chemistry, Myongji University, Korea*

A practical conversion method of monomeric carbohydrates into heterocyclic compounds was developed by the reaction with amino acid and oxalic acid in dry DMSO at 90°C based on Maillard reaction. The mild Maillard variant of carbohydrates and amino acid in heated DMSO with oxalic acid expeditiously produced the pyrrole-2-carbaldehyde skeleton. Further cyclization of the highly functionalized Pyrralines afforded the pyrrole-fused poly-heterocyclic compounds as potential lead compounds for drugs ,food flavors, and functional materials.



Poster Presentation : **ORGN.P-509**

Organic Chemistry

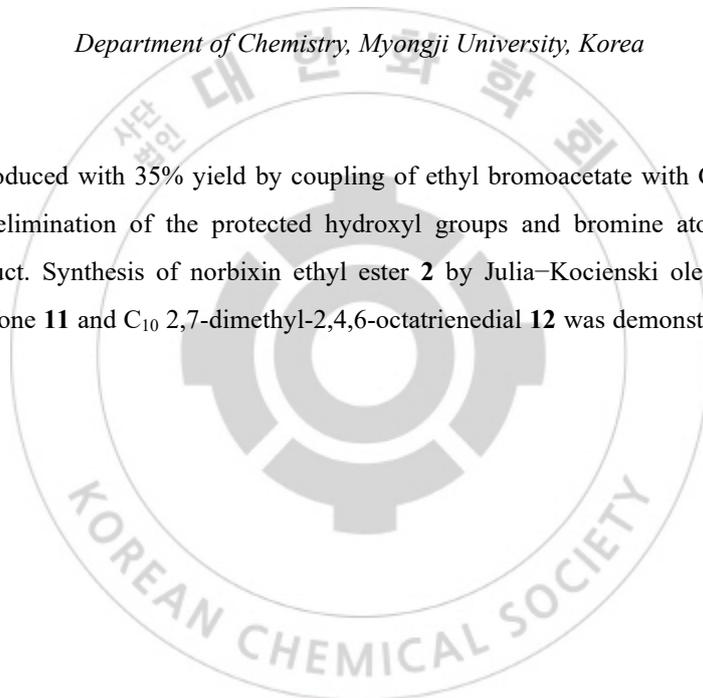
Zoom 12 FRI 16:00~17:00

Synthesis of Norbixin and Its Ester by a Practical Bromoacetate and Julia–Kocienski Olefination

Aleksei Golikov, Sangho Koo*

Department of Chemistry, Myongji University, Korea

Norbixin **1** was produced with 35% yield by coupling of ethyl bromoacetate with C₂₀ dialdehyde **6** and following double elimination of the protected hydroxyl groups and bromine atoms of the coupling bromohydrin product. Synthesis of norbixin ethyl ester **2** by Julia–Kocienski olefination of novel C₇ benzothiazolyl-sulfone **11** and C₁₀ 2,7-dimethyl-2,4,6-octatrienedial **12** was demonstrated with 36% yield overall.



Poster Presentation : **ORGN.P-510**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

GSH-responsive nanoparticles based on porphyrin-betulinic acid conjugates for photodynamic therapy

Mengyao Yang, Juyoung Yoon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

Photodynamic therapy (PDT) has become a promising treatment modality over conventional therapies due to its features. However, the efficacy of PDT is severely limited on account of inherent shortcomings of PDT (e.g., limited depth of light penetration) and the lack of tumor specific photosensitizers (PSs) that can be tackled by designing of activated PSs through usage of stimuli responsive delivery systems. Herein, a GSH-responsive nanoparticle (NanoP-ss-BA) has been designed by linking the porphyrin derivative (P) to the naturally occurring betulinic acid (BA) through a disulphide bond. NanoP-ss-BA could be triggered disassembly by GSH and effectively promotes singlet oxygen (1O_2) production, and also releases lipophilic anticancer drug, BA in situ, which serve NanoP-ss-BA as a good candidate for PDT.

Poster Presentation : **ORGN.P-511**

Organic Chemistry

Zoom 12 FRI 16:00~17:00

Direct Preparation of Azido Compounds and C-C Bond from Allyl Protected Alcohols using Catalytic AlCl_3

Tien Tan Bui, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

Alcohols are easily protected by allyl group, and frequently observed as form of allylic ethers in many organic syntheses. Direct preparations of azido compounds and nucleophilic substituted compounds from allyl-protected alcohols is attractive study due to reduction of cost, time, and waste. In this study, a series of catalysts was tested to discover the optimal reaction conditions for the direct reaction of benzyl allyl ethers, and it is found that AlCl_3 was the most appropriate catalyst for direct preparation of azido compounds from benzyl allyl ethers, and TMSN_3 was a good azido reagent. In this reaction method using AlCl_3 , and TMSN_3 , various azido compounds were successfully synthesized from the reaction of benzyl allyl ethers in good yield. Furthermore, direct C-C bond formation was achieved *via* reaction of benzyl allyl ethers with carbon nucleophiles and AlCl_3 . The result proved that novel AlCl_3 -catalyzed reaction procedures of allyl-protected alcohol can result in successful reactions including azidation, allylation, and alkynylation.

Poster Presentation : **ORGN.P-512**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Phthalocyanine/albumin self-assembly for acid-activated fluorescence imaging, and photodynamic immunotherapy

Rui Wang, Juyoung Yoon*

Department of Chemistry and Nanoscience, Ewha Womans University, Korea

We here reported activatable albumin-phthalocyanine nanoassembly complex, NPc1, it can not only kill tumor cells directly by producing a broad of toxic ROS but also provoke immune responses by increasing tumor-related antigens to T cells. Pc1 as the monomer structure is composed of two parts, silicon phthalocyanine as the backbone and morpholine which is modified on the silicon phthalocyanine axis. NPc1 exhibited bright near-infrared fluorescence under acidic conditions circumstances that promote the ability to target tumors. More significantly, NPc1 combined with α -PD-1 checkpoint blockade can eliminate primary tumors after NIR laser irradiation on the one hand, on the other hand, abscopal effects inhibited the distant tumor even metastatic tumor via long-term immune memory.

Poster Presentation : **ORGN.P-513**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

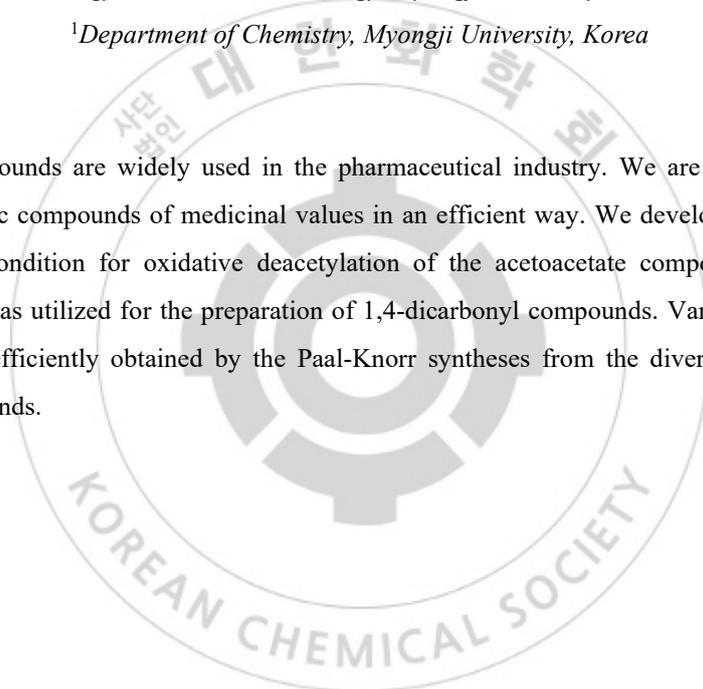
Synthesis of native products via Mn/Co catalytic system

Miao Zhang, Sangho Koo^{1,*}

Energy Science and Technology, Myungji University, Korea

¹*Department of Chemistry, Myungji University, Korea*

Heterocyclic compounds are widely used in the pharmaceutical industry. We are trying to synthesize various heterocyclic compounds of medicinal values in an efficient way. We developed a very effective Mn/Co catalytic condition for oxidative deacetylation of the acetoacetate compounds under aerobic condition, which was utilized for the preparation of 1,4-dicarbonyl compounds. Various hetero-aromatic compounds were efficiently obtained by the Paal-Knorr syntheses from the diversely substituted 1,4-dicarbonyl compounds.



Poster Presentation : **ORGN.P-514**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Fast Assembly and High-Throughput Screening of Structure and Antioxidant Relationship of Carotenoids

Gaosheng Shi, Sangho Koo^{1,*}

Department of Energy Science and Technology, Myongji 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-515**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

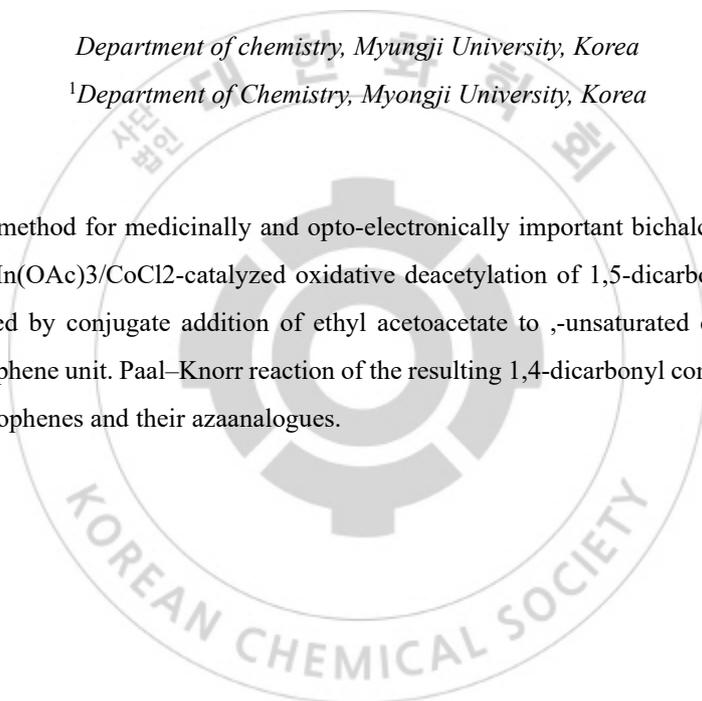
Synthesis of Biologically Active Heterocyclic Compounds by Mn(III)-catalyzed Radical Oxidation

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.



Poster Presentation : **ORGN.P-516**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Regioselective functionalization of glycerol

Chanyoung Boo, Hyein Kim, Sangho Koo^{1,*}

Department of Chemistry, Myungji University, Korea

¹*Department of Chemistry, Myongji University, Korea*

We studied the regio-selective functionalization of propane-1,2,3-triol (glycerol). Carboxylic acid and phenol were respectively and regio-selectively attached to glycerol to produce 1,3- and 1,2-diglycerides. First, phenol was reacted with epichlorohydrin under basic condition to give etherification product, which then underwent regio-selective ring opening reaction with carboxylic acids at the less hindered carbon of epoxide to give 1,3-diglycerides. On the other hand, 1,2-diglycerides were prepared through the above 1,3-diglyceride of acetic acid, which required tri-glyceride synthesis by Steglich esterification with carboxylic acids at the 2-position (free secondary OH), followed by deprotection of the acetyl group at the 3-position.

Poster Presentation : **ORGN.P-517**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Nanoparticle Fe₂O₃-catalyzed Friedel-Crafts Acylation of Aromatic Substrates

Tien Tan Bui, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

Aromatic ketones are the important intermediates for preparation of compounds with broad applications including pharmaceuticals, agrochemicals, fragrances, and dyes. Over the years, Friedel-Crafts acylation has been usually employed to synthesize these aryl ketones *via* Bronsted acids or Lewis acids. However, there are several drawbacks in the conventional methods such as the use of stoichiometric amounts of catalysts, and unrecyclable reagents due to their consumption in the reaction, which led to environmentally hazardous procedures. Therefore, the environmental-friendly conversion of acyl halide to generate corresponding aryl ketones is greatly demanded. In this study, we developed a novel, mild and efficient formation of aryl ketones from acyl bromide in the presence of nanoparticle Fe₂O₃ in solvent-free condition. A wide scope of aryl ketones was prepared in high yield and the catalyst could be recycled within this transformation. The result presented that the direct preparation of acyl bromide to aromatic ketones is highly effective process and can be exploited in many organic syntheses.

Poster Presentation : **ORGN.P-518**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Silane based symmetric EBL materials for efficient OLED application

Subin Oh, Younghee Park*, Kanthasamy Raagulan*, Jinsoo Ghim*, Kyu Yun Chai^{1,*}

Department of chemistry, Wonkwang University, Korea

¹Department of Chemistry, Wonkwang University, Korea

In this study a new electron injection control layer material was synthesized through Suzuki reaction with silane-based material as the starting material. The compound synthesized is N-(4-(2-(4-((4-(9-(4-(diphenylamino)phenyl)-9H-carbazol-2-yl)phenyl)diphenylsilyl)phenyl)-9H-carbazol-9-yl)phenyl)-N-phenylbenzenamine(S-1), N-(4-(2-(4-((4-(9-(4-(diphenylamino)phenyl)-9H-carbazol-2-yl)phenyl)dimethylsilyl)phenyl)-9H-carbazol-9-yl)phenyl)-N-phenylbenzenamine(S-2). The synthesized compound showed excellent ability as an electron injection control layer material due to its ability to transmit perforation and transport perforation, and it was found that it was measured most similar to TCTA material, and the device was produced using TCTA material as a reference. The new electronic injection control layer materials, S-1, S-2, all showed excellent thermal and morphological stability due to their bulky molecular structure. S-1, S-2 showed the same turn on voltage result as TCTA (2.6V), while driving voltage was 5.6V and 5.7V lower than TCTA (6.0V). The current and voltage efficiency of S-1 is 75.9/75.1cd/A and the external quantum efficiency is 31.1/31.0%. The current and voltage efficiency of S-2 is 72.6/71.8 cd/A, with an external quantum efficiency of 27.9/27.7%, and higher than TCTA (69.4/65.1 cd/A, 25.3/24.2%). As a result, excellent device element performance was confirmed.

Poster Presentation : **ORGN.P-519**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Direct Synthesis of Asymmetric Ureas from *N*-Alloc- and *N*-Troc - Protected Amines using Lanthanum (III) Trifluoromethanesulfonate

Tien Tan Bui, Hee-Kwon Kim*

Department of Nuclear Medicine, Jeonbuk National University, Korea

Urea is one of the most common moieties in many substances with broad applications such as pharmaceuticals, organic materials, and natural products. While many preparations of urea motif have been developed over years, conventional synthetic methods still exist several drawbacks including unstable intermediates or toxic phosgene as reagent. Allyloxycarbonyl (Alloc-) and 2,2,2-Trichloroethoxycarbonyl (Troc-) were employed as protecting groups to prevent side reactions of amine group in organic reactions,. Therefore, the direct transformation of *N*-Alloc- and *N*-Troc-protected amines to ureas is promising pathway. In this study, various rare-earth triflate salts were investigated as the catalyst to generate urea compounds from *N*-Alloc- and *N*-Troc-protected amines. In screening, lanthanum (III) trifluoromethanesulfonate played as effective catalyst of this transformation. Moreover, the higher conversion yields of urea compounds were observed in trifluorotoluene. With these optimal reaction conditions, various aromatic and aliphatic ureas were synthesized from corresponding *N*-Alloc- and *N*-Troc-protected amines in excellent yield. The result suggested that the direct conversion of *N*-Alloc- and *N*-Troc-protected amines to urea compounds using lanthanum trifluoromethanesulfonate is highly useful procedure and can be applied in an array of organic syntheses.

Poster Presentation : **ORGN.P-520**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Acridine based high triplet energy small molecular hole transport type materials for phosphorescent OLED application

Youngee Park, Subin Oh^{*}, Jinsoo Ghim^{*}, Kanthasamy Raagulan^{*}, Kyu Yun Chai^{1,*}

Department of chemistry, Wonkwang University, Korea

¹*Department of Chemistry, Wonkwang University, Korea*

Two small molecular hole transporting type materials, namely 4-(9,9-dimethylacridin-10(9H)-yl)-N-(4-(9,9-dimethylacridin-10(9H)-yl)phenyl)-N-phenylaniline (TPA-2ACR) and 10,10'-(9-phenyl-9H-carbazole-3,6-diyl)bis(9,9-dimethyl-9,10-dihydroacridine) (PhCAR-2ACR) were designed and synthesized by single step Buchwald-Hartwig amination between dimethyl acridine and triphenylamine or carbazole core. Both materials showed high thermal decomposition temperature of 380 and 422 °C at 5% weight reduction for PhCAR-2ACR and TPA-2ACR, respectively. The triplet energy of the material was around 3 eV, and which support an effective energy flow to the dopant. TPA-2ACR as hole transporting material exhibited excellent current, power, and external quantum efficiencies of 55.74 cd/A, 29.28 lm/W and 21.59%, respectively and which values are much higher than that of reference 1,1-Bis[(di-4-tolylamino)phenyl]cyclohexane (TAPC) based similar device (32.53 cd/A, 18.58 lm/W and 10.6%). Phenyl carbazole based PhCAR-2ACR showed good device characteristics as host materials when compare to reference 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP), and the current and external quantum efficiencies were 56.90 cd/A and 20.57%, 47.83 cd/A and 18.16%, respectively. This efficiency is better than that of our reference materials in the same application.

Poster Presentation : **ORGN.P-521**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

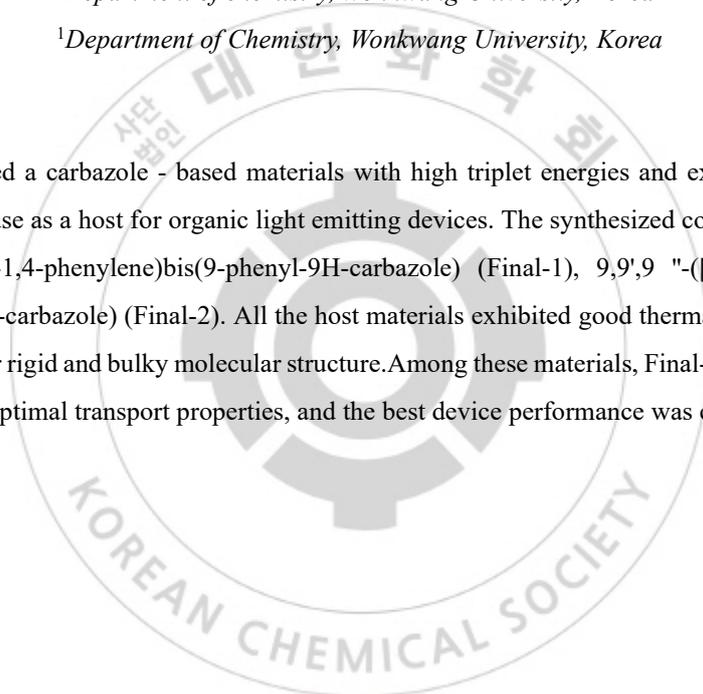
Carbazole based hole transporting type materials for OLEDs.

Jinsoo Ghim, Subin Oh^{*}, Younghee Park^{*}, Kanthasamy Raagulan^{*}, Kyu Yun Chai^{1,*}

Department of chemistry, Wonkwang University, Korea

¹*Department of Chemistry, Wonkwang University, Korea*

we have synthesized a carbazole - based materials with high triplet energies and excellent hole transfer characteristics for use as a host for organic light emitting devices. The synthesized compounds are 3,3'-(2-(9H-carbazol-9-yl)-1,4-phenylene)bis(9-phenyl-9H-carbazole) (Final-1), 9,9,9'-([1,1':4',1''-terphenyl]-2',4,4''-triy)tris(9H-carbazole) (Final-2). All the host materials exhibited good thermal and morphological stability due to their rigid and bulky molecular structure. Among these materials, Final-1 showed the highest triplet energy and optimal transport properties, and the best device performance was confirmed.



Poster Presentation : **ORGN.P-522**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

DDQ-Catalyzed Aerobic Oxidative Allylation of Benzyl Ethers

Sujin Lee, Sun-Joon Min^{1,*}

Applied Chemistry, Hanyang University, Korea

¹*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) is a versatile and powerful oxidant that has been used as a stoichiometric reagent in numerous organic reactions. Nevertheless, the stoichiometric use of DDQ often causes purification difficulties in large-scale syntheses and has some toxicity concerns. To solve this problem, an alternative catalytic combination of a stoichiometric amount of a terminal oxidant and DDQ has been proposed. However, most of them offer little benefit because they use an excess of metal-based oxidant to oxidize the corresponding hydroquinone to DDQ. Several oxidants such as NaNO_2 , HNO_3 are suggested as alternatives and TBN (tert-butyl nitrite) is currently used as one of the most attractive reagents for this purpose. In this study, we present metal-free oxidative allylation of benzyl ether using DDQ/TBN co-catalyst system for activation of benzylic C-H bond. This synthetic method could be applied to the synthesis of a variety of oxacyclic compounds such as tetrahydrofuran or tetrahydropyran derivatives. Our effort to optimize the reaction conditions and investigate the scope of substrates will be described in this presentation.

Poster Presentation : **ORGN.P-523**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Palladium-Catalyzed Aerobic Benzannulation of Pyrazoles with Alkynes

Jae Yeong Song, Jung Min Joo*

Department of Chemistry, Pusan National University, Korea

The Pd-catalyzed C–H benzannulation of heteroarenes with alkynes has been performed to access heteroarene-containing extended π -systems by using stoichiometric metal oxidants. However, these metal oxidants, such as Ag(I) and Cu(II) salts, are expensive and toxic. As a sustainable approach, we developed Pd-catalyzed annulation reactions of pyrazoles using oxygen as the oxidant. Under the optimized aerobic conditions, pyrazoles were reacted with various aryl alkynes to afford tetraaryl substituted indazoles. To further compare the aerobic and Cu-mediated methods, 1:1 annulation reactions with phenylpyrazoles and alkynes were conducted to show the advantage of the aerobic method. This green approach will allow the synthesis of indazoles in a single step and facilitate their applications as organic fluorescent materials.



Poster Presentation : **ORGN.P-524**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

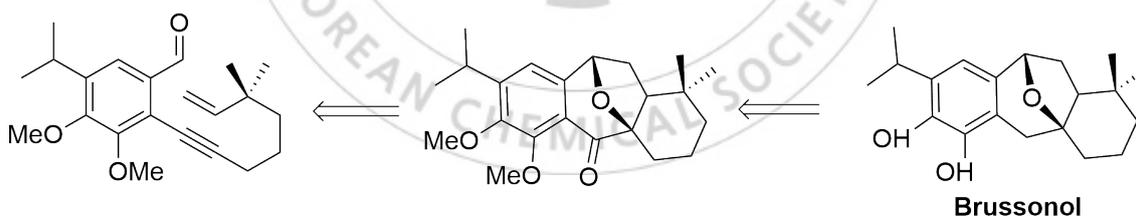
Synthesis of Brussonol by use a Gold-catalyzed Cyclization Reaction

Le Thuy Quynh, Chang Ho Oh^{1,*}

Chemistry department, Hanyang University, Korea

¹*Department of Chemistry, Hanyang University, Korea*

The transition-metal catalyzed cyclization of unsaturated compound brings efficient and environmentally friendly method to synthesis of natural products. Recently, we reported the construction of [6,7,6] tricyclic skeletons by using transition-metal catalyzed cyclization (Au, Pt..), which as key intermediates for synthesis icetaxane-diterpenoid (faveline, komaroviquinone, taxamairin B and rosmaridiphenol). Herein, we will provide an efficient synthesis to construct the [6,7,6] tricyclic- key skeletons which could be applied to the construction of icetaxanes as representing Brussonol. The possible reaction mechanisms have been proposed.



Poster Presentation : **ORGN.P-525**

Organic Chemistry

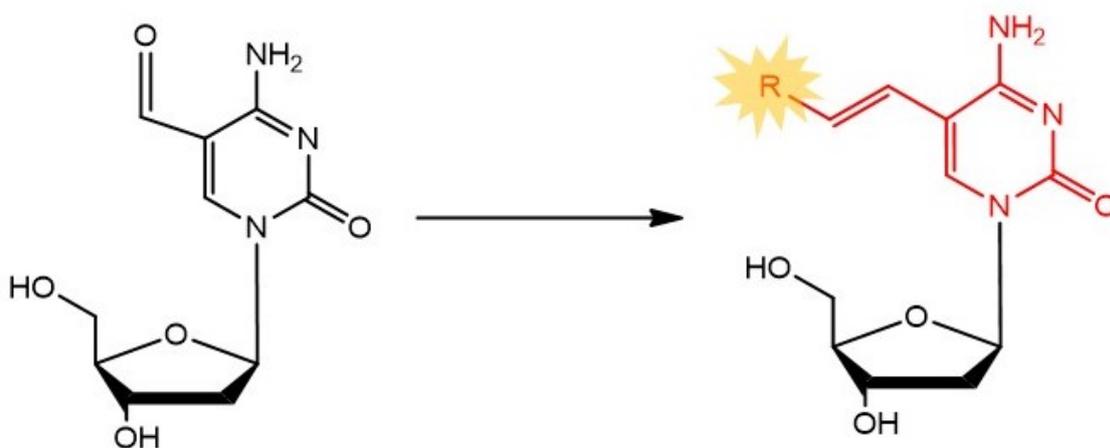
Zoom 13 FRI 15:00~16:00

Design and synthesis of novel fluorescent nucleosides derived from 5-formylcytosine

Hayeon Choi, Hokyung Kim, Ki Tae Kim*

Department of Chemistry, Chungbuk National 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 high fluorescence quantum yields, brightness, and environmental sensitivity has become an important challenge. Herein, we report a synthetic strategy for novel fluorescent nucleosides, based on diverse reactions of 5-formylcytosine (5-fC). High reactivity and broad reaction scope of the formyl group in 5-fC enabled construction of push-pull type fluorescent nucleosides, exhibiting large Stokes shift as well as high brightness, which are useful for designing improved version of nucleic acid systems.



Poster Presentation : ORGN.P-526

Organic Chemistry

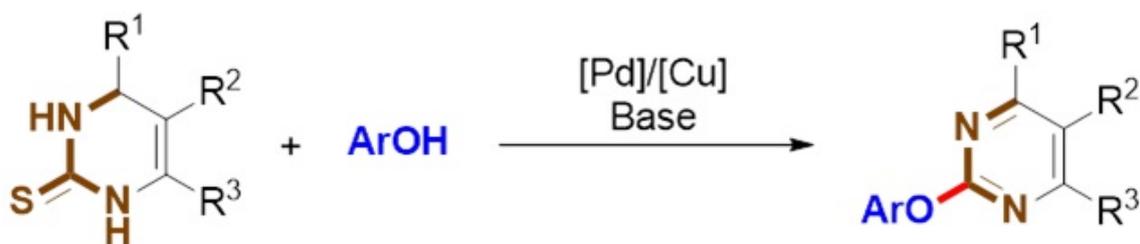
Zoom 13 FRI 15:00~16:00

Oxidative Dehydrosulfurative Carbon-oxygen Cross-coupling of 3,4-Dihydropyrimidine-2-thiones with Aryl Alcohols

Jihong Lee, Jeong-Hun Sohn*

Department of Chemistry, Chungnam National University, Korea

We present a Pd-catalyzed/Cu-mediated oxidative dehydrosulfurative carbon-oxygen cross-coupling reaction of 3,4-dihydropyrimidin-1*H*-2-thiones (DHPMs) with aryl alcohols. Due to the ready availability of diverse DHPMs and aryl alcohols,¹ the reaction method offers facile access to biologically and pharmacologically valuable 2-aryloxy pyrimidine derivatives with rapid diversification.²**References**1. (a) Singh, K.; Singh, K. *Adv. Heterocycl. Chem.* **2012**, *105*, 223-308. (b) Suresh; Sandhu, J. S. *ARKIVOC* **2012**, 66-133. (c) Patil, R. V.; Chavan, J. U.; Dalal, D. S.; Shinde, V. S.; Beldar, A. G. *ACS Comb. Sci.* **2019**, *21*, 3, 105-148.2. (a) Kang, F. A.; Kodah, J.; Guan, Q.; Li, X.; Murray, W. V. *J. Org. Chem.* **2005**, *70*, 1957-1960. (b) Wang, Y. -F.; Liu, W. -M.; Zhu, Y. -Q.; Zou, X. -M.; Hu, F. -Z.; Yang, H. -Z. *J. Heterocyclic Chem.* **2006**, *43*, 1275-1280. (c) Venu, T. D.; Khanum, S. A.; Firdouse, A.; Manuprasad, B. K.; Shashikanth, S.; Mohamed, R.; Vishwanth, B. S. *Bioorg. Med. Chem. Lett.* **2008**, *18*, 4409-4412. (d) Wang, X. C.; Yang, G. J.; Jia, X. D.; Zhang, Z.; Da, Y. X.; Quan, Z. *J. Tetrahedron*, **2011**, *67*, 3267-3272. (e) Quan, Z.; Jing, F.; Zhang, Z.; Da, Y.; Wang, X. *Chin. J. Chem.* **2013**, *31*, 1495-1502. (f) Walsh, K.; Sneddon, H. F.; Moody, C. J. *RSC Adv.* **2014**, *4*, 28072-28077. (g) Meng, J. -P.; Wang, W. -W.; Chen, Y. -L.; Bera, S.; Wu, *J. Org. Chem. Front.* **2020**, *7*, 267-272.



Poster Presentation : **ORGN.P-527**

Organic Chemistry

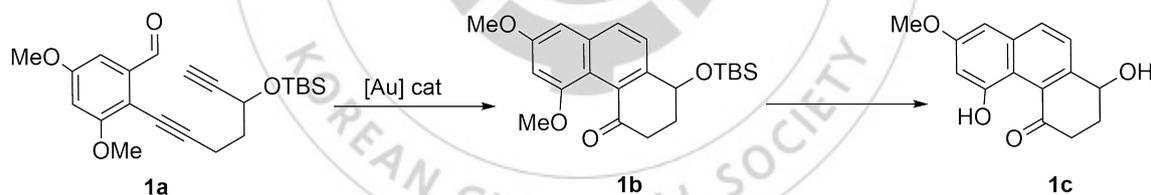
Zoom 13 FRI 15:00~16:00

Synthesis of [6,6,6] polycyclic compound Dendrodevonin A and its derivatives

Seunghwan Ham, Juyeon Kang, Chang Ho Oh*

Department of Chemistry, Hanyang University, Korea

The natural product dendrodevonin series have been isolated from the stem of *Dendrobium devonianum*. A series of aromatic compounds, including phenanthrenes, bibenzyls, flavones and simple aromatic acids and esters, have attracted the attention of many organic chemists for their diverse biological activities. We have successfully synthesized dendrodevonin A 1c and its derivatives from diyne substrates 1a via intramolecular [4+2] cycloaddition by transition metal catalysts.



Scheme 1. Synthesis of Dendrodevonin A 1c from diyne substrate 1a.

Poster Presentation : **ORGN.P-528**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Late-stage $^{18}\text{F}/^{19}\text{F}$ Isotopic Exchange to Produce Aryl ^{18}F Fluorosulfates and Sulfamoyl ^{18}F Fluorides without Azeotropic Drying

MinJu Lee, Sungwon Jun, Joong-Hyun Chun*

Department of Nuclear Medicine, Yonsei University College of Medicine, Korea

Recent advances in sulfur (VI) fluoride exchange chemistry have yielded vast chemical libraries used in the pharmaceutical, materials science, and agrochemical industries. Furthermore, isotopic activation of different sulfonyl groups with fluorine-18 provides new possibilities for drug discovery. There are multiple unmet needs in the drug development process that require expedient ^{18}F - labeling of various aryl fluorosulfates and sulfamoyl fluorides. To this end, we have developed a method for rapid isotopic exchange at the sulfonyl core between fluorine-19 and radioactive fluorine-18. To overcome the limitations incurred from the short physical half-life of fluorine-18 ($t_{1/2} = 110$ min), the usual azeotropic drying process (10–20 min) was excluded. Various aryl ^{18}F fluorosulfates and sulfamoyl ^{18}F fluorides were obtained by $^{18}\text{F}/^{19}\text{F}$ isotopic exchange with cyclotron-produced ^{18}F fluoride ion. Unlike aryl ^{18}F fluorosulfates, which were accessed directly from phenols, sulfamoyl ^{18}F fluorides were inaccessible, or only accessible in low yields, from their corresponding amines. Herein, we report a late-stage $^{18}\text{F}/^{19}\text{F}$ isotopic exchange protocol that affords various ^{18}F -labeled aryl fluorosulfates and sulfamoyl fluorides at radiochemical yields up to 92%, as determined by radio-HPLC analyses. This labeling protocol provides an efficient and alternative route for incorporating ^{18}F into sulfur–oxygen and sulfur–nitrogen compounds, enabling the development of a diverse chemical library based on the sulfonyl core. This work was funded by the National Research Foundation (NRF-2019R1F1A1058774) of Korea.

Poster Presentation : **ORGN.P-529**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Synthesis of indole derivatives as inhibitors of acetylcholinesterase and butyrylcholinesterase.

Seungyeon Lee, Kooyeon Lee*

Department of Bio-Health Convergence, Kangwon National University, Korea

The enzymes acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) are key targets of cholinergic disorders. A series of indole derivatives were designed, synthesized and evaluated for inhibitory activities against cholinesterase (ChE). Because the indole nucleus is a privileged structural motif that has been found in a vast number of alkaloid natural products and of synthetic molecules with significant biological activities. The ChE inhibitory activity studies were carried out using Ellman's colorimetric method. Most of the tested compounds exhibited inhibitory activity against AChE and BuChE. Among them **1m** showed the highest AChE inhibitory activity with the IC_{50} value of 30.3 μ M, especially compound **1l** and **1m** exhibited the highest BuChE inhibitory activity with the IC_{50} value of 0.6 μ M. Thus, these derivatives could be further developed to provide novel leads for the discovery of new anti-Alzheimer drugs in the future.

Poster Presentation : **ORGN.P-530**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

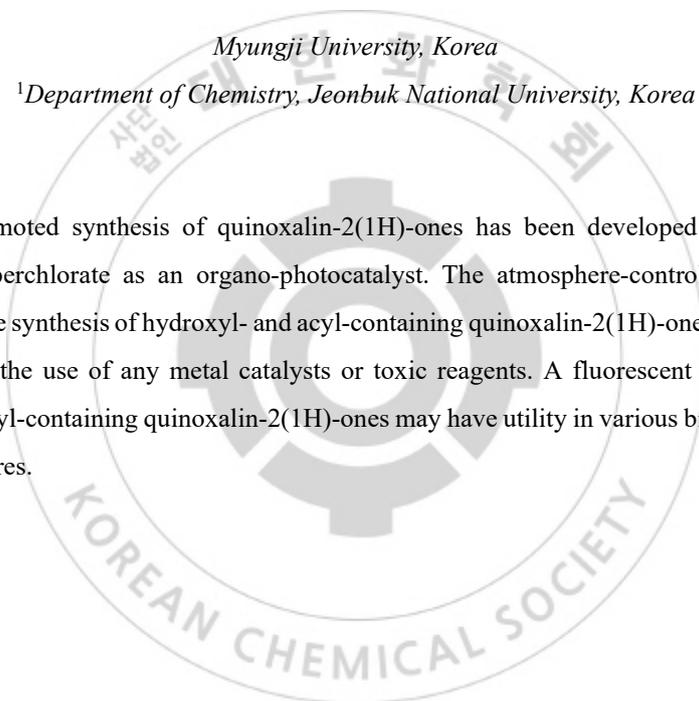
Visible-Light-Promoted Switchable Synthesis of C-3-Functionalized Quinoxalin-2(1H)-ones

Kim Christopher Aganda, Anna Lee^{1,*}

Myungji University, Korea

¹*Department of Chemistry, Jeonbuk National University, Korea*

A visible-light-promoted synthesis of quinoxalin-2(1H)-ones has been developed using 9-mesityl-10-methylacridinium perchlorate as an organo-photocatalyst. The atmosphere-controlled method (Ar/air) enabled the selective synthesis of hydroxyl- and acyl-containing quinoxalin-2(1H)-ones under mild reaction conditions without the use of any metal catalysts or toxic reagents. A fluorescent labelling experiment showed that hydroxyl-containing quinoxalin-2(1H)-ones may have utility in various biological applications as potent fluorophores.



Poster Presentation : **ORGN.P-531**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Hydrophobic Superacid Catalysis to Access α -Tertiary-Amines “On-Water”

Sungyeon Cho, Han Yong Bae*

Department of Chemistry, Sungkyunkwan University, Korea

A tetrasubstituted carbon atom connected by three carbons with single nitrogen, i.e., α -tertiary amine (ATA) functional group, is an essential building block incorporated in naturally occurring alkaloids and pharmaceuticals. Although a limited number of catalytic processes to access this moiety via amination or 1,2-addition reactions have been reported, however, still fewer are commonly utilized in the practical syntheses. This is perhaps due to the difficulty of preparing starting material, which is elaborately designed to utilize a key catalysis step. We report herein a remarkably powerful catalytic method to access ATA moiety, exploiting abundant natural ketone feedstocks as useful starting material. More interestingly, a hydrophobic superacid catalyst enables the facile formation of challenging ATA moiety under the “on-water” condition. The unconventional catalytic condition in the multi-component allylation system facilitates extremely broad substrate scope and efficient multi-gram scalability. Conventional organic solution conditions or less hydrophobic acid catalysts failed to achieve the highly selective transformation due to the lower reactivity or considerable by-products generation.

Poster Presentation : **ORGN.P-532**

Organic Chemistry

Zoom 13 FRI 15:00~16:00

Designing Foldamer Building Blocks for Supramolecular Coordination Assemblies

Jaewook Kim, Jintaek Gong¹, Hee-Seung Lee*

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

¹Center for Multiscale Chiral Architectures, Korea Advanced Institute of Science and Technology, Korea

Supramolecular coordination assemblies have been treated as useful materials in numerous applications. However, the building blocks of these well-organized assemblies mostly contain aromatic moieties for rigid architectures. Therefore, the demand for a new type of building blocks has risen to overcome the weakness of aromatic ligands. In this research, we designed non-aromatic foldamer ligands composed of α -amino acid with metal-binding site and 2-aminocyclopentanecarboxylic acid (ACPC) monomer. The ACPC monomers are well-known to help the foldamer fold in a rigid helical structure which makes the metal-binding sites locate on desired position and gives us an advantage to control the geometry of the assembled architectures. Based on the design, we synthesized hexameric foldamers with the combination of ACPC and α -amino acid monomers. We determined their molecular structures and tested their metal-binding affinity. The result clearly showed that the designed foldamers have potential to be used as building blocks for supramolecular coordination assemblies.

Poster Presentation : **ORGN.P-533**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Modular Construction of Chain Molecules with Fluorescent Repeats and Sharp Turns

Suk-il Kang, Sungmin Song, Hongsik Kim, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

To exploit fluorophores for energy transfer, molecular switching, and chemical sensing, it is important to develop molecular platforms, in which the fluorophores are structurally and electronically well-defined. Toward this objective, we built a series of zig-zag-shaped π -conjugated oligomers having fluorescent tolane units that are oriented parallel to each other across bis(triazolo)benzene-based turn motifs. A comparative computational study revealed that steric constraints imposed by the side chains play a critical functional role in enforcing the desired folded conformation. A combination of photophysical and DFT computational studies established that the bis(triazolo)benzene motifs electronically disjoint the fluorophores, so that they behave as independent light-absorbing and -emitting units. This presentation will discuss key design principles, synthetic implementations, and practical implications of this previously unknown class of π -conjugated chain molecules.

Poster Presentation : ORGN.P-534

Organic Chemistry

Zoom 13 FRI 16:00~17:00

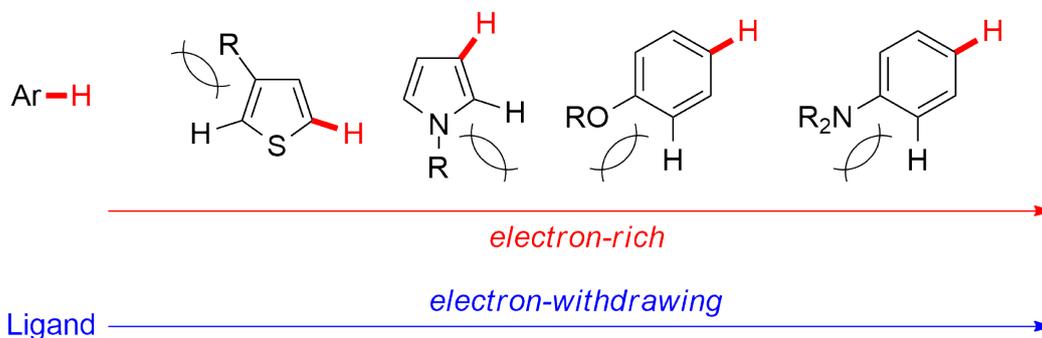
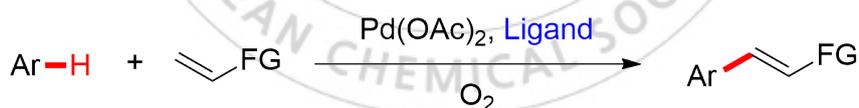
Sterically Controlled C–H Alkenylation of (Hetero)arenes Using Pyrazolonaphthyridine Ligands

Eunsu Kang, Jung Min Joo^{1,*}

Department of chemistry, Pusan National University, Korea

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

Carefully matched coupling strategies using transition metals and ligands are essential for the development of successful direct C–H activation reactions. The newly designed nitrogen bidentate ligands, pyrazolonaphthyridine (PzNPy) ligands were applied to the Pd-catalyzed regioselective alkenylation of (hetero)arenes. The pyrazole core, which is less Lewis basic than pyridine, enabled the alkenylation of electron-rich arenes and the oxidation of Pd(0) species under O₂ conditions without any additional oxidants. The effects of ligands on the reaction rate and selectivity will be discussed based on the structure of Pd(II)-ligand complexes and their binding strength studies.



Poster Presentation : **ORGN.P-535**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

A BODIPY-based Fluorescent Probe for the Detection of Tyrosinase Activity

Siyoung Cho, Youngmi Kim*

Department of Chemistry, Kyung Hee University, Korea

Tyrosinase, which is found in melanocytes in plant and animal tissues, plays an important role in melanin synthesis. However, inhibition of tyrosinase expression causes severe skin diseases such as oculocutaneous albinism type I, which is a symptom of albino and overexpression of this enzyme occurs melanoma. It also acts on dopamine neurotoxicity and neurodegeneration associated with Parkinson's disease. Therefore, the development of sensitive and selective probes for the detection of tyrosinase activity would be very important. Recently, we have reported that controlling the photophysical properties of *meso*-substituted-1,3,5,7-tetramethyl-BODIPY dyes by introducing different functional groups at *meso*-position. In particular, the conversion of a *meso*-ester of 1,3,5,7-tetramethyl-BODIPY dyes to the corresponding *meso*-carboxylate derivatives leads to significant changes in fluorescence properties of the dyes. By taking advantage of these features, we have designed the *meso*-substituted-1,3,5,7-BODIPY incorporating recognition moiety for tyrosinase. We synthesized a probe **A** that can selectively detect tyrosinase. Probe **A**, before reaction with tyrosinase, showed a weak fluorescence due to the steric effect by methyl groups at 1,7-positions. Upon incubation with tyrosinase, probe **A** is converted to *meso*-carboxylate via R1 group is leaving. This conversion results in large spectral changes: red-shifted absorption and emission bands (λ_{abs} :563 nm, λ_{emi} :586 nm) and a large turn-on signal (~35-fold). Probe **A** also exhibits high stability (upto 6 h) as well as excellent selectivity for tyrosinase over other bio-related species. Our new probe can be applied for the detection of tyrosinase in human disease.

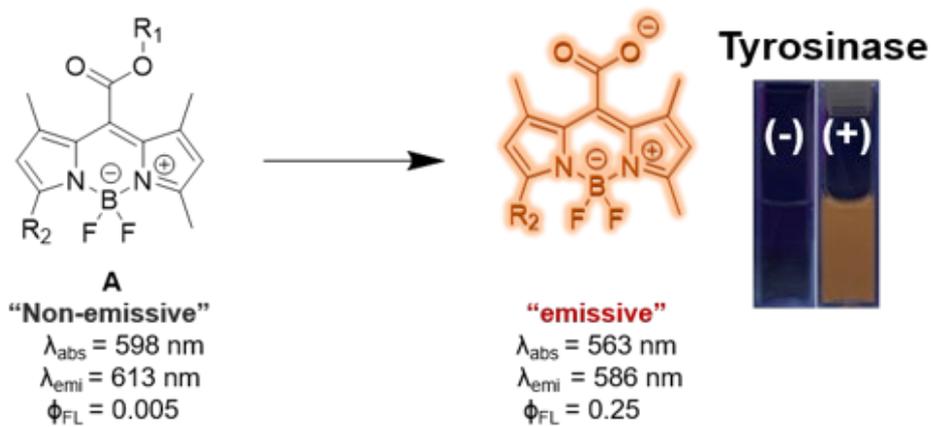


Figure 1. Design of compound **A** and the proposed sensing mechanism.



Poster Presentation : **ORGN.P-536**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Hydrogen Bonding-Guided Assembly of Columnar π -Stacks: Conformationally Rigid Molecular Clips for Self-Association and Host–Guest Chemistry

Hyun Lee, Dongwhan Lee*

Department of Chemistry, Seoul National University, Korea

Columnar π -stack structures have potentials as electronic and optical materials. For the applicability, precise molecular-level control of columnar π -stacks is an important prerequisite to define conduits for excitons or charge-carriers. To make vertically stacked multi-layer aromatics with well-defined orientation and spatial ordering, we have designed and synthesized a series of C-shaped molecules having spatially preorganized π -surfaces. These molecules have shape complementary van der Waals (vdW) surfaces and hydrogen bonds that synergistically reinforce each other for sequence-selective self-dimerization to afford quadruple π -stacks in the solution phase. In the solid state, “inter”dimer π – π stacking assists a hierarchical growth of discrete dimers into an infinite columnar structure. For a homologous series of regioisomers built with three different pyrenyl substituents, a subtle difference in the π – π arrangements led to dramatic changes in the self-association constant. The underlying molecular mechanism of this shape-dependent property was investigated by a combination of X-ray crystallographic and NMR spectroscopic studies. The C-shaped cavity can also take up a small-sized flat aromatic molecule to form a host–guest complex as triple π -stacks. This presentation will discuss key principles of conformational design and synergistic non-covalent interactions to realize self-organizing π -stacks with an extraordinary level of fidelity in long-range structural ordering.

Poster Presentation : **ORGN.P-537**

Organic Chemistry

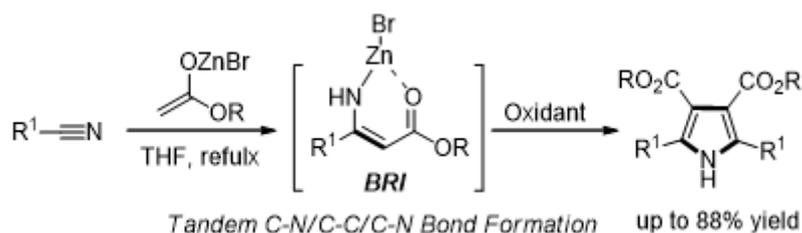
Zoom 13 FRI 16:00~17:00

Tandem One-Pot Synthesis of Tetrasubstituted NH Pyrroles via Oxidative Dimerization of the Zinc Bromide Complex of β -Enamino Esters

HyeongSu Kim, Juhyun Kim*, Zi Xuan*

Department of Chemistry, Gyeongsang National University, Korea

Tetrasubstituted *N*-H pyrrole has attracted extensive attention in the field of biology, medicine, material science and dye industry. Accordingly, recent diverse approach on the synthesis of pyrroles such as transition metal catalyzed reactions, dipolar cycloaddition, oxidative cross coupling reactions have been developed. Despite of these improvement, efficient methodologies toward the pyrroles are still in highly demand if the reaction runs in tandem one-pot manner from simple starting materials without isolation of intermediate. Blaise reaction intermediate (BRI) which is zinc bromide complex of β -enaminoesters forms from simple nitriles with Reformatsky reagent is an useful and chemically applicable intermediate for the synthesis of versatile heterocyclic compounds^[1]. Herein, we proposed tandem one-pot synthesis of tetrasubstituted *N*-H pyrroles by using via Blaise reaction / oxidative dimerization / cyclization reaction from simple nitriles.^[1] Kim, J. H, Ko, Y. O, Bouffard, J, Lee, S.-g, *Chem. Soc. Rev.*, **2015**, 44, 2489-2507



Poster Presentation : **ORGN.P-538**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

C=S bond based heavy-atom-free photosensitizers for hypoxia photodynamic therapy and ClO⁻ detection

Thanh Chung Pham, Songyi Lee^{1,*}

Department Interdisciplinary Program of Biomedical, Mechanical and Electrical Engineering, Korea

¹*Department of Chemistry, Pukyong National University, Korea*

Photodynamic therapy (PDT) is one of the attractive alternatives to conventional cancer treatment using photosensitizers (PSs). A photosensitizer exhibited negligible dark cytotoxicity, but irradiation of a PS in the presence of molecular oxygen promotes the formation of reactive oxygen species (ROS) through a type I or type II process, causing cytotoxicity. Among many PSs, only small amount of them have been efficiently applied in cancer PDT treatment under hypoxia condition. On the other hand, lots of research have been focused on developing selective fluorescent probes to image ROS/RNS including ClO⁻, H₂O₂, NO, ONOO⁻, •O₂⁻, 1O₂ and biothiols. To understand the critical roles of ClO⁻, monitoring and imaging the location of ClO⁻ at the live cells are essential. We designed and synthesized the thionated NpImidazole derivatives BS and NS, new heavy-atom-free photosensitizers, which efficiently generates triplet excited states with high singlet oxygen quantum yields. The introduction of C=S bond to NpImidazole core is essential for increasing spin-orbit coupling (SOC). The fluorescence emission of BS and NS were quenched at room temperature, accompanying with the enhancement of ISC process from the singlet to triplet excited state via thionation. BS and NS showed negligible dark cytotoxicity against HeLa cells in working concentration. In the contrast, BS and NS rapidly induced cell death under blue light irradiation both in normoxia and hypoxia condition. Our current study demonstrates that C=S group can play an important role in type I ROS generation of PSs, which have unprecedented in the previous reports. Finally, the photophysical changes was assigned to the oxidative desulfurization of C=S group of BS and NS to C=O group of the corresponding BO and NO via hypochlorite. The combined results demonstrated the dual function of BS and NS as a fluorescent imaging agent for ClO⁻ and an anti-cancer therapeutic by PDT that showed the potential strategy for “one-for-all” as well as multifunctional agents.



Poster Presentation : **ORGN.P-539**

Organic Chemistry

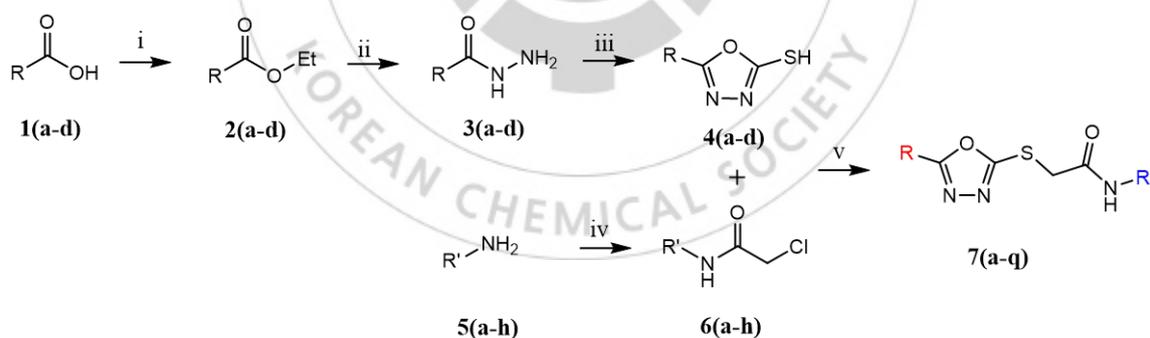
Zoom 13 FRI 16:00~17:00

Novel oxadiazole-amide derivatives inhibit the carbonic anhydrase level

Nam Gyu Choi, Ki Hwan Lee*

Department of Chemistry, Kongju National University, Korea

In this research work, oxadiazole and amide derivatives were synthesized and characterized. The carbonic anhydrase inhibitor potential of the target compounds was assessed. Amongst the 17 synthesized compounds, the compounds(7f, 7g, 7n, 7o) demonstrate an excellent carbonic anhydrase inhibitory activity. Especially, the compound **7g**($IC_{50} = 0.076 \pm 0.009 \mu\text{M}$) confirms much more significant potent inhibition activity compared with standard substance acetazolamide ($IC_{50} = 1.09 \pm 0.073 \mu\text{M}$).



Poster Presentation : **ORGN.P-540**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Polysaccharide film as a template for interfacial chemistry

Young Jae Jung, JungKyu Lee^{1,*}

Chemistry, Kyungpook National University, Korea

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

As a polysaccharide agarose is a linear polymer, consisting of alternating D-galactose and 3,6-anhydro-L-galactopyranose units.[1] As a gel, agarose has been commonly used as a template in biology for nucleic acid and protein analysis, cell culture, recombinant virus titration due to its biopassivity, biocompatibility, and simple preparation. In recent, agarose film, formed by the dehydration of agarose gel, has emerged as a versatile scaffold for a functionalizable, non-biofouling material because of its transparency, micrometer-scale thickness, and strong mechanical strength upon adhesion to surfaces.[2] In this presentation, we will discuss the preparation, characterization, and chemical functionalization of agarose film and cover few examples of applications, such as protein and cellular patterning as well as colorimetric assay for protein and metal ion.[3][1] J. O. Jeppson; C. B. Laurell; Bi Franzen. *Clinical Chemistry*. 1979, 25, 629–638. [2] G. Han; D. Hong; B. S. Lee; E. Ha; J. H. Park; I. S. Choi; S. M. Kang; J. K. Lee. *Chem. Asian J.* 2017, 12, 846-852[3] H. W. Kim; Y. J. Jung; J. K. Lee. *Polym. Chem. DOJ*: 10.1039/d0py01616k.

Poster Presentation : **ORGN.P-541**

Organic Chemistry

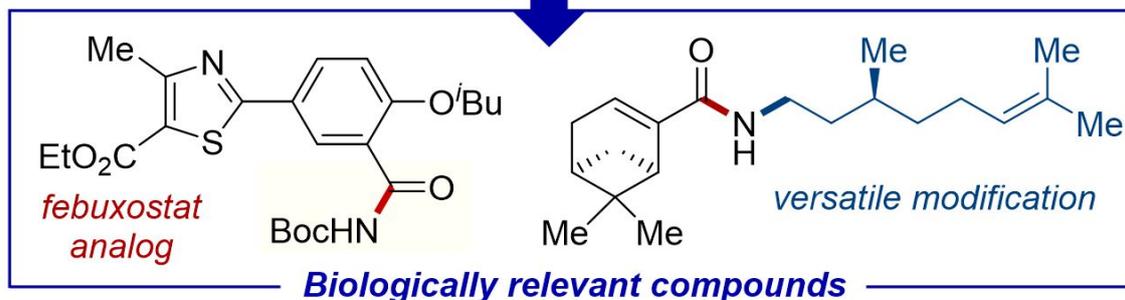
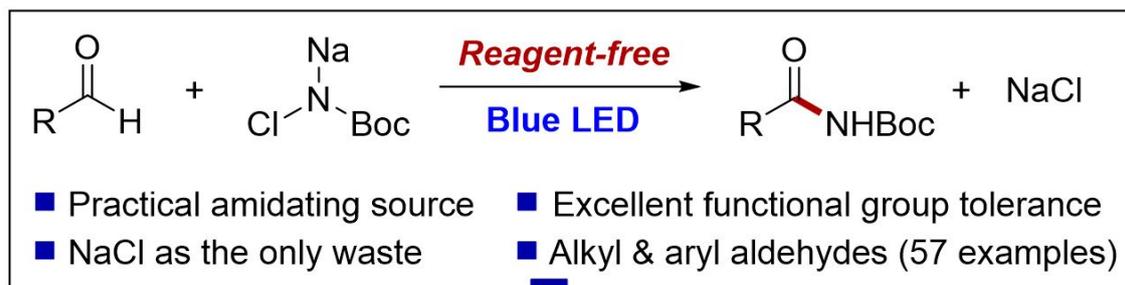
Zoom 13 FRI 16:00~17:00

Controlled Relay Process to Access N-Centered Radicals for Catalyst-free Amidation of Aldehydes under Visible Light

Wongyu Lee, Sukbok Chang*

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

Amides are an important class of structural motifs prevalently found in Nature, such as proteins, peptides and bioactive natural products. Furthermore, the combination of their high stability and interesting physical properties has led to the widespread applications in material science, medicinal chemistry and chemical biology. Therefore, the development of applicable amidation reactions from alternative functional moieties is highly sought after, as this would provide diversity for the synthesis of chemical entities that are inaccessible through the conventional approach. Here, we developed a visible-light-induced approach for amidation of aldehydes, utilizing *N*-chloro-*N*-sodio-carbamate as a catalyst-free amidation reagent to afford *N*-protected amides under mild and convenient conditions. This synthetic operation relies on an unconventional relay process to convert aldehydes to amides under the catalyst, oxidant and coupling reagents-free conditions, which is enabled by the development of a new mechanistic platform that gives efficient and controllable access to *N*-centered radicals under visible light. A wide range of (hetero)aromatic and aliphatic aldehydes can be employed, including those derived from biologically relevant complex molecules. We anticipate that the accomplished methodological advances, combined with the unique mechanistic features, will lead to the widespread application of the present strategy in broad research fields.



Poster Presentation : **ORGN.P-542**

Organic Chemistry

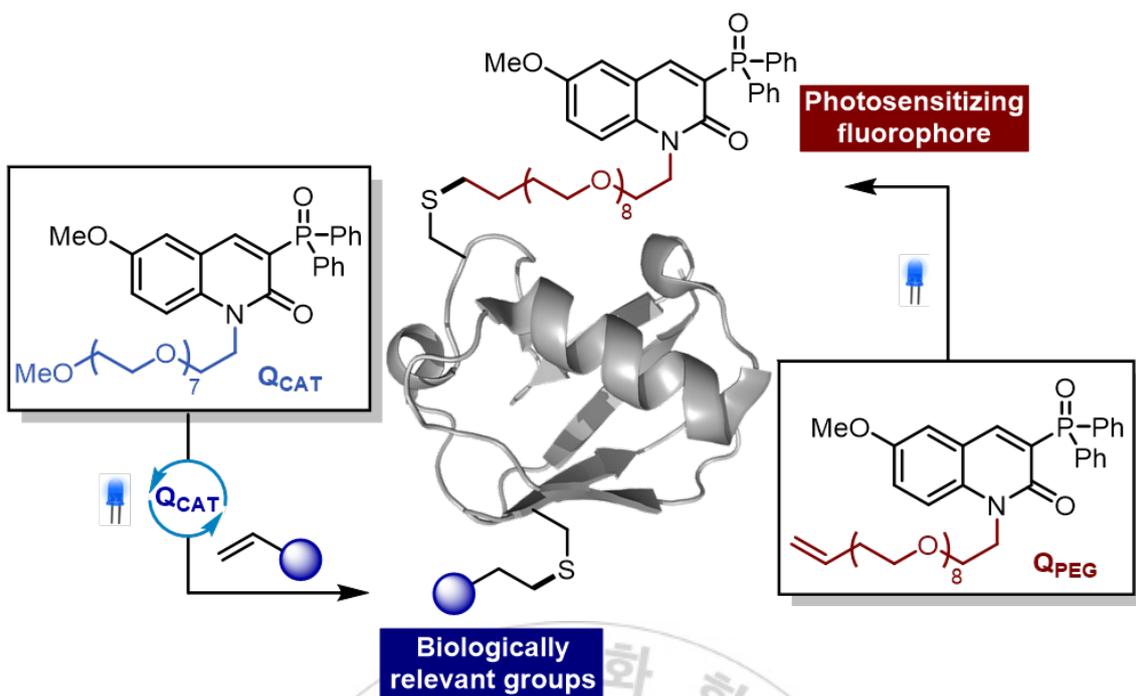
Zoom 13 FRI 16:00~17:00

Visible-Light-Induced Cysteine-Specific Bioconjugation: Biocompatible Thiol-Ene Click Chemistry

Hangyeol Choi, Myojeong Kim, Sungwoo Hong*

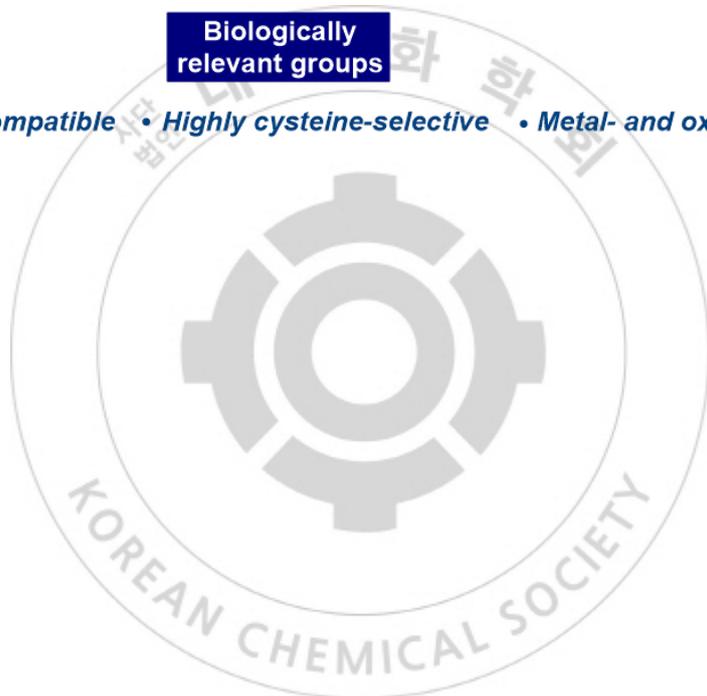
Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Bioconjugation methods using visible-light photocatalysis have emerged as powerful synthetic tools for the selective modification of biomolecules under mild reaction conditions. However, the number of photochemical transformations that allow successful protein bioconjugation is still limited because of the need for stringent reaction conditions. Herein, we report that a newly developed water-compatible fluorescent photosensitizer QPEG can be used for visible-light-induced cysteine-specific bioconjugation for the installation of QPEG by exploiting its intrinsic photosensitizing ability to activate the S–H bond of cysteine. The slightly modified QCAT enables the effective photocatalytic cysteine-specific conjugation of biologically relevant groups. The superior reactivity and cysteine selectivity of this methodology was further corroborated by traceless bioconjugation with a series of complex peptides and proteins under biocompatible conditions.



Biologically relevant groups

- *Water-compatible*
- *Highly cysteine-selective*
- *Metal- and oxidant-free*



Poster Presentation : **ORGN.P-543**

Organic Chemistry

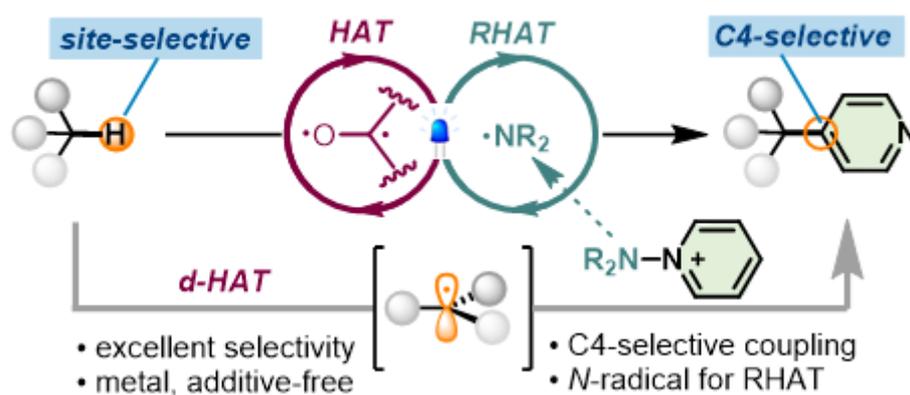
Zoom 13 FRI 16:00~17:00

Site-Selective Direct C–H Pyridylation of Unactivated Alkanes Enabled by Anthraquinone and N-Aminopyridinium Salts

Wooseok Lee, Sungwoo Hong*

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

Site-selective functionalization of C–H bonds using visible light is a challenging and useful reaction in the broad field of chemical research. We report 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. N-aminopyridinium salts achieved the selective pyridylation of more substituted, electron-rich C–H bonds in abundant chemical feedstocks. 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.



Poster Presentation : **ORGN.P-544**

Organic Chemistry

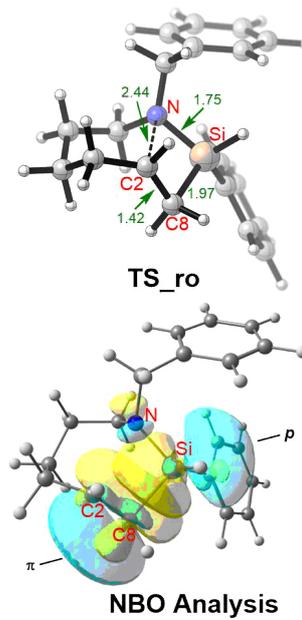
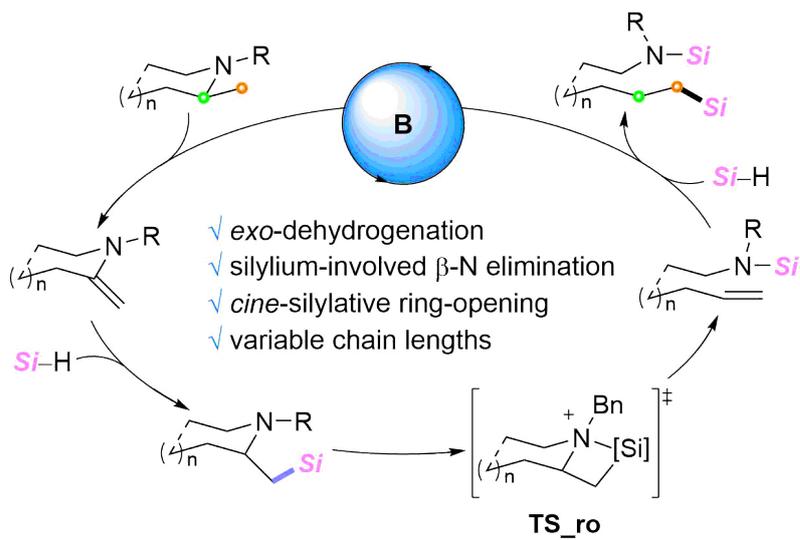
Zoom 13 FRI 16:00~17:00

***cine*-Silylative Ring-Opening of α -Methyl Azacycles Enabled by the Silylium-Induced C–N Bond Cleavage**

Sukbok Chang^{*}, Jianbo Zhang

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

N-Heterocyclic compounds are widely presented as a key component of numerous natural products, pharmaceuticals and materials. Readily available saturated azacycles such as pyrrolidine and piperidine are versatile synthetic building units allowing an installation of functional groups into the cyclic skeletons. As a complementary strategy, deconstructive functionalization of N-heterocycles has also drawn an increasing interest in recent years. This approach provides acyclic amines tethered with remote functional groups. Despite the notable skeletal reorganization associated with the deconstructive transformation, it often suffers from unsatisfactory regioselectivity and poor functional group tolerance due to the oxidative reaction conditions. While an *ipso*-functionalized ring-cleavage of N-heterocycles can be achieved by masking the nitrogen atom with suitable protecting groups, the deconstruction of alicyclic amines incorporating organic groups adjacent to the C–N bond (*cine*-substitution) remains highly challenging. Described herein is the development of a borane-catalyzed *cine*-silylative ring-opening of α -methyl azacycles. This transformation involves four-step cascade processes: (i) *exo*-dehydrogenation of alicyclic amine, (ii) hydrosilylation of resultant enamine, (iii) silylium-induced *cis*- β -amino elimination to open the ring skeleton, and (iv) hydrosilylation of terminal olefin. This procedure offers an unprecedented approach towards the synthesis of α,ω -aminosilanes that are tethered with variable carbon chains, and cleavage of C–N bond of acyclic tertiary amines efficiently. On the basis of integrated experimental and computational studies, the silicon atom was elucidated to play a pivotal role in the β -amino elimination step.



Poster Presentation : **ORGN.P-545**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Tuning Triplet Energy Transfer of Hydroxamates as the Nitrene Precursor for Intramolecular C(sp³)-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. We reported the design of a photosensitization strategy to generate triplet nitrenes and their applicability for the intramolecular C-H amidation reactions. Substrate optimization by tuning triplet energy and reorganization 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. Mechanism studies supported our working hypothesis that the energy transfer path is mainly operative.

Poster Presentation : **ORGN.P-546**

Organic Chemistry

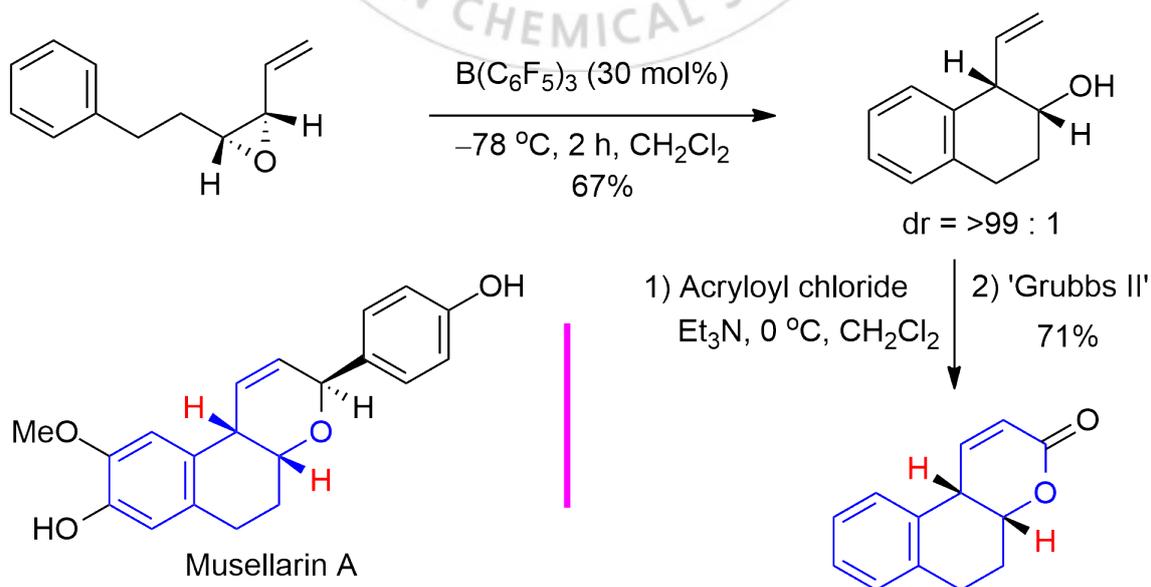
Zoom 13 FRI 16:00~17:00

A Carbocyclization of Vinyloxiranes Catalyzed by Lewis Acids for the Construction of the Musellarin Tricyclic Core

Sehui Yang, Euijin Park, Jimin Kim*

Department of Chemistry, Chonnam National University, Korea

Vinyloxiranes have become versatile building blocks due to their unique reactivity arising from the combination of the vinyl and the epoxide. A number of reactions using these epoxides have accumulated over the past years including radical and cycloaddition reactions as well as nucleophilic openings. Various nucleophiles are introduced to the openings of vinyloxiranes, and one of the nucleophiles is electron-rich pi system as a carbon nucleophile. We would like to present herein several crucial points that have emerged during our recent investigations for carbocyclizations of vinyloxiranes catalyzed by Lewis acids to provide cyclic homoallyl alcohols as single isomers: 1) the choice of Lewis acid, $B(C_6F_5)_3$ was crucial for the stereoselective transformation in the case of cis vinyloxiranes, whereas $BF_3 \cdot OEt_2$ was proven to be an effective catalyst for trans substrates.



Poster Presentation : **ORGN.P-547**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Amide to Nitrile Conversion with Vilsmeier Reagent after C-H Bond Functionalizations

Haneul Yoo, Dopil Kim¹, Min Kim^{1,*}

Chungbuk National University, Korea

¹*Department of Chemistry, Chungbuk National University, Korea*

Directing group (DG) chemistry is a key strategy for selective C-H bond functionalizations with transition metals. Various DGs have been studied for regioselective C-H bond functionalizations through metal-coordination and C-H bond activations.¹ However, DGs generally require the installation steps and the additional removal process from the substrates. Therefore, ease elimination of DGs and/or transformation of DGs after C-H bond functionalization have many attentions in recent years.

Amide group is very efficient DG for *ortho* C-H bond functionalizations with various transition metals such as Pd, Ir, Ru, and Rh. Although the installation of amide is quite simple, the removal process of amide or transformation of amide are very restricted due to their low reactivity.² In this presentation, the conversion of amides to corresponding nitriles with Vilsmeier reagent will be discussed. Especially, this simple transformation could be adopted just after transition metal-catalyzed C-H bond functionalizations reaction. Detail reaction conditions and substrate scopes will be presented.

References1. Sambigiato, C.; Schonbauer, D.; Blicke, R.; Dao-Huy, T.; Pototschnig, G.; Schaaf, P.; Wiesinger, T.; Zia, M. F.; Wencel-Delord, J.; Besset, T.; Maes, B. U. W.; Schnurch, M. *Chem. Soc. Rev.* **2018**, *47*, 6603.2. Zhu, R.-Y.; Farmer, M. E.; Chen, Y.-Q.; Yu, J.-Q. *Angew. Chem. Int. Ed.* **2016**, *55*, 10578.

Poster Presentation : **ORGN.P-548**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Selective Carbonyl-Ene Reactions by Metal-Organic Framework Catalysts

Dopil Kim, Nakcheol Jeong^{1,*}, Min Kim^{*}

Department of Chemistry, Chungbuk National University, Korea

¹*Department of Chemistry, Korea University, Korea*

Metal-organic frameworks (MOFs) are versatile platform for catalytic organic reactions. The fine-tunability and perfect heterogeneity allowed various strategies and catalyst loadings for organic transformations. In addition, their unique 3-dimensional porous structure gives a restricted reaction environment. Therefore, the substrate size selectivity and stereoselectivity controls have been achieved through MOF-based catalysts.¹

Recently, binol-based KUMOF-1 was reported, and following metalation with Zn and Ti gave efficient and selective catalyst for carbonyl-ene reactions.² In this study, the differences of reaction behavior between Zn-mediated carbonyl-ene reaction and Ti-catalyzed carbonyl-ene reactions were mainly studied. In case of Ti, the major reaction was occurred at the surface of MOF crystal, the stereoselectivity was not fully controlled by MOF pores.

In this presentation, the recent progress on the size-selective and stereo-selective KUMOF catalyst for carbonyl-ene reactions will be discussed. The mixed ligand strategy and surface-deactivation method were mainly introduced into KUMOF catalyst.

References

- 1) S. Jeoung, S. Kim, M. Kim, H.R. Moon, *Coord. Chem. Rev.* **2020**, *420*, 213377.
- 2) J. Han, M.S. Lee, P.K. Thallapally, M. Kim, N. Jeong, *ACS Catal.* **2019**, *9*, 3969.

Poster Presentation : **ORGN.P-549**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Pd-catalyzed γ site-selective C-H arylation with transient directing groups

Hyeon Bin Ha, HoJeong Choi, Jaesung Kwak¹, Byunghyuck Jung², Min Kim*

Department of Chemistry, Chungbuk National University, Korea

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

²*Department of Emerging Materials Science, Daegu Gyeongbuk Institute of Science & Technology, Korea*

Hyeonbin Ha, Ho Jeong Choi, Jaesung Kwak*, Byunghyuck Jung*, Min Kim*

Transient directing groups (TDGs, or temporary directing groups) is practical strategy to introduce site- and regio-selectivity for transition metal-catalyzed organic reactions. Although traditional directing groups (DGs) require the installation and removal steps for the substrate, the TDGs are prepared through reversible reaction under *in situ* manner. The imine-based TDGs from aldehyde substrate and amine ligand or amine substrate and aldehyde ligand have been widely studied for various transition metal-catalyzed organic reactions.¹

In this presentation, our recent studies for palladium-catalyzed γ -selective C-H bond activation for arylation of aliphatic amines will be discussed.² The C-H bond functionalization of free aliphatic amines are relatively restricted due to the nature of amine group (metal coordinating ability, basicity, redox chemistry, and etc). Therefore, the TDG strategy with aldehyde-based TDG for imine formation is very efficient way to direct C-H functionalization of aliphatic amine substrate. In addition, the perfect site-selectivity was also achieved. The catalytic reaction screening along with substrate scope will be presented.

References 1. Gandeepan, P.; Ackermann, L. *Chem*, **2018**, *4*, 199. 2. Ha, H.; Choi, H. J.; Park, H.; Gwon, Y.; Lee, J.; Kwak, J.; Kim, M.; Jung, B. *Eur. J. Org. Chem.* **2021**, *Early View*.

DOI:10.1002/ejoc.202001428

Poster Presentation : **ORGN.P-550**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Degradation property of surface-modified porous silicon nanostructure in biological media

Rae Hyung Kang, Dokyoung Kim^{1,*}

Biomedical Science, Kyung Hee University, Korea

¹*College of Medicine, Kyung Hee University, Korea*

Recently, porous silicon nanoparticles (pSiNP) have been investigated in biomedical fields including nanomedicine and biosensors due to their biocompatibility, intrinsic near-infrared (NIR) photoluminescence, and high loading efficiency. In addition, the surface-functionalized pSiNP is imperative in enhancing their properties and usage; (i) hydrophobicity/hydrophilicity balance control in order to improve water dispersibility and drug loading efficiency, (ii) release profile control, and (iii) the introduction of the targeting moiety to cell/organ/bacteria. However, the biodegradation rate of surface-functionalized pSiNP formulations in different biological media has not been known. In this study, we prepared four different surface-functionalized pSiNP; (i) pSiNPs-F: surface-functionalized with FITC-PEG, in order to simply analysis the degradation rate of pSiNP, (ii) pSiNPs-F-mPEG: surface-functionalized with FITC-PEG/methoxy-terminal PEG (iii) pSiNP-F-NHS: surface-functionalized with FITC-PEG/N-hydroxysuccimide (NHS)-terminal PEG, (iv) pSiNP-F-MAL: surface-functionalized with FITC-PEG/maleimide (MAL)-terminal PEG. Next, we characterized the particle properties such as structural morphology and size, zeta-potential, and functional groups on surface of nanoparticles and systematic analyzed the degradation rate in six different biological media; (i) deionized water (DI H₂O), (ii) phosphate-buffered saline (PBS), (iii) Dulbecco's modified Eagle's medium (DMEM); cell culture media, (iv) human serum (HS), (v) lysogeny broth (LB); bacteria culture media, and (vi) brain heart infusion (BHI); microorganism culture media. We suggested that our results provide useful insights in designing the new surface-functionalized pSiNP formulation for various biomedical applications.

Poster Presentation : **ORGN.P-551**

Organic Chemistry

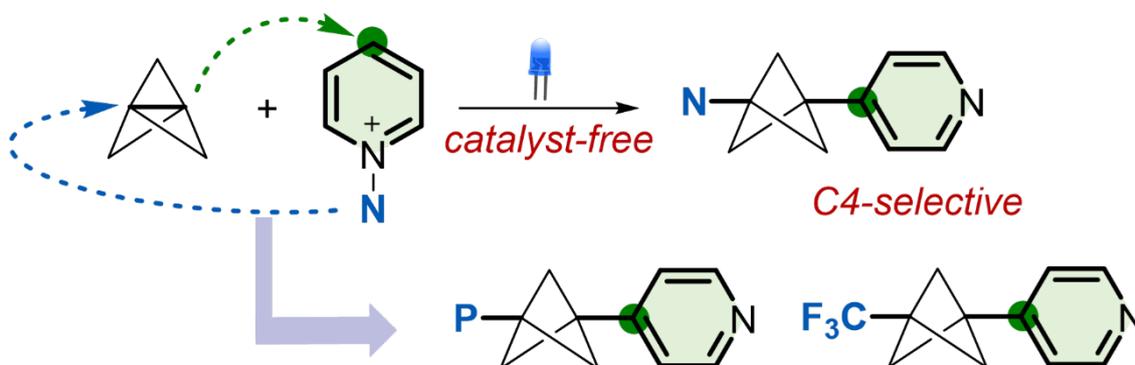
Zoom 13 FRI 16:00~17:00

Strain-Release Pyridylation of [1.1.1]Propellanes Using N-Aminopyridinium Salts with Electrophilic Radicals Under Visible Light Irradiation

Sanghoon Shin, Sungwoo Hong*

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

We have successfully achieved the strain-release pyridylation of [1.1.1]propellane using N-aminopyridinium salts. With the aid of an EDA electron donor–acceptor (EDA) complex, we could get bicyclo[1.1.1]pentane (BCP) frameworks without requiring a photocatalyst under blue LEDs irradiation. This method exhibits a wide range of substrate scopes and high functional-group tolerance to afford 1,3-aminopyridylated BCPs under mild and metal-free conditions. The late-stage functionalization of complex compounds further demonstrates the applicability of this method. The synthetic utility could be extended to other electrophilic radicals such as phosphinoyl and trifluoromethyl radicals for the direct incorporation to the BCP core, offering divergence via a three-component assembly. Overall, this protocol lays the approach for the straightforward synthesis of new valuable pyridylated BCP motifs, remarkably extend the scope of BCP-type bioisosteres for drug design applications.



Poster Presentation : **ORGN.P-552**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Synthesis of polynitrogen compound for energetic materials

Hae-Wook Yoo^{*}, Kuktae Kwon, SeungHee Kim, So Jung Lee

Agency for Defense Development, Korea

High energy density materials (HEDMs) are used to determine the final performance in various weapon systems developed for military purposes like as explosives and propellant. High explosive substances represented by TNT and RDX are well-known high energy materials and they consist mainly of derivatives of cyclic compounds containing nitrogen. In the case of nitrogen-containing molecules, very stable triple bonded N₂ molecules are formed during the decomposition process. There is a large difference in energy level, and therefore, the development of high-energy materials is mainly focused on the development of molecules with high nitrogen content. However, due to the high stability of the N₂ molecule, synthesis of polynitrogen compounds is quite difficult and often exhibits the property of being easily decomposed. Up to now, the synthesis of high energy molecules based on triazole and tetrazole has been actively progressing. Recently, a study on a pentazole compound, a form of polynitrogen, which is drawing attention as an ultimate high energy material, has been published. In this study, we recognized the necessity of securing the technology for synthesizing pentazole compounds and confirmed the possibility of synthesis of the pentazole compound on a laboratory scale.

Poster Presentation : **ORGN.P-553**

Organic Chemistry

Zoom 13 FRI 16:00~17:00

Tuning Orbital Symmetry of Iridium Nitrenoid Enables Catalytic Diastereo- and Enantioselective Alkene Difunctionalizations

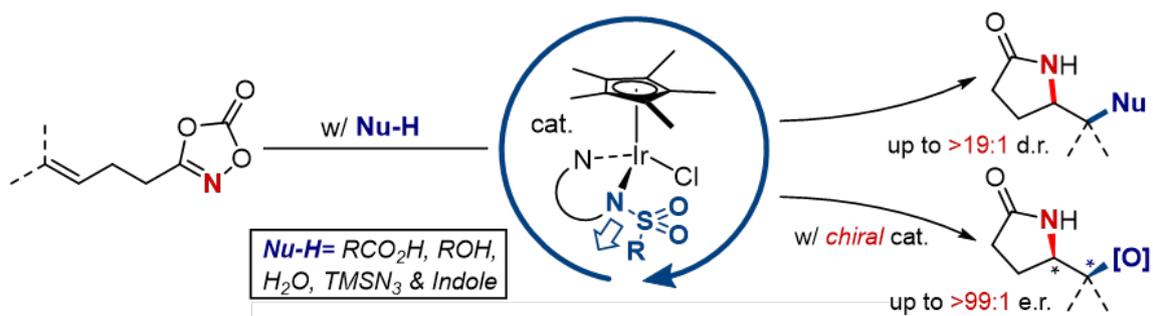
Suhyeon Kim, Dongwook Kim¹, Seung Youn Hong^{2,*}, Sukbok Chang^{*}

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

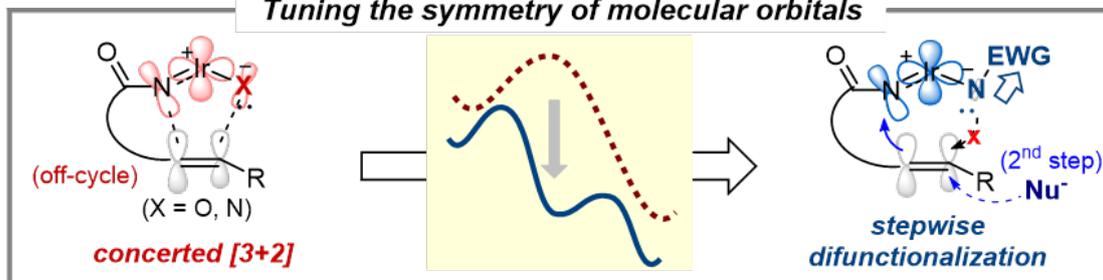
¹*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

²*Department of Chemistry, Massachusetts Institute of Technology, United States*

Among the central themes in synthetic chemistry is to establish novel strategies that usher in the development of more efficient and mild reactions, and also expand the chemical space for asymmetric catalysis. Herein, we present an approach to revitalize the Cp*Ir(κ_2 -LX) system as a catalyst toward alkene difunctionalizations via nitrenoid-mediated pathway. A key strategy is tuning orbital symmetry of the key Ir-nitrenoid intermediates by the ligand modification to impart the desired catalytic activity with the suppression of catalyst deactivation. Based on the frontier molecular orbital (FMO) analysis, we systematically engineered a new catalyst system capable of a stepwise nitrenoid transfer to allow for nucleophile incorporation. Using the catalytic protocol, a range of difunctionalized lactams can be produced in a diastereoselective manner with various nucleophiles. Mechanistic investigations revealed that the ligand plays a crucial role in both nitrenoid delivery and stereoselectivity-determining steps. The current mechanistic platform also enabled the development of new asymmetric methods for introducing two-point chirality in (oxy-alkyl)lactam products with excellent enantioselectivity.



Tuning the symmetry of molecular orbitals



Poster Presentation : **ORGN.P-554**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

i-Motif DNA probes bearing N,N-dimethylaminofluorene-labeled 2'-deoxyuridine unit.

Seung Woo Hong, Gil Tae Hwang*

Department of Chemistry, Kyungpook National University, Korea

In our previous study, N,N-dimethylaminofluorene-labeled 2'-deoxyuridine (U^{DAF}) was incorporated into the central position of 2'-deoxyoligonucleotides (ODNs). ODNs increased their fluorescent emission property with lowered pH value. In this study, we inserted U^{DAF} into a thymine position of human telomeric (hTelo) i-motif sequence. i-motif is a DNA structure found in C-rich area at acidic pH. Therefore, we could investigate the correlation between pH value and emission property. Emission intensity of i-motif sequence was gradually increased as their pH value diminished. Furthermore, thermal stability, CD spectra, and UV absorbance were investigated. With these results, we determined pH_m to set the i-motif structure unfolding point. Studies on hTelo i-motif sequence with different U^{DAF} position are underway.

Poster Presentation : **ORGN.P-555**

Organic Chemistry

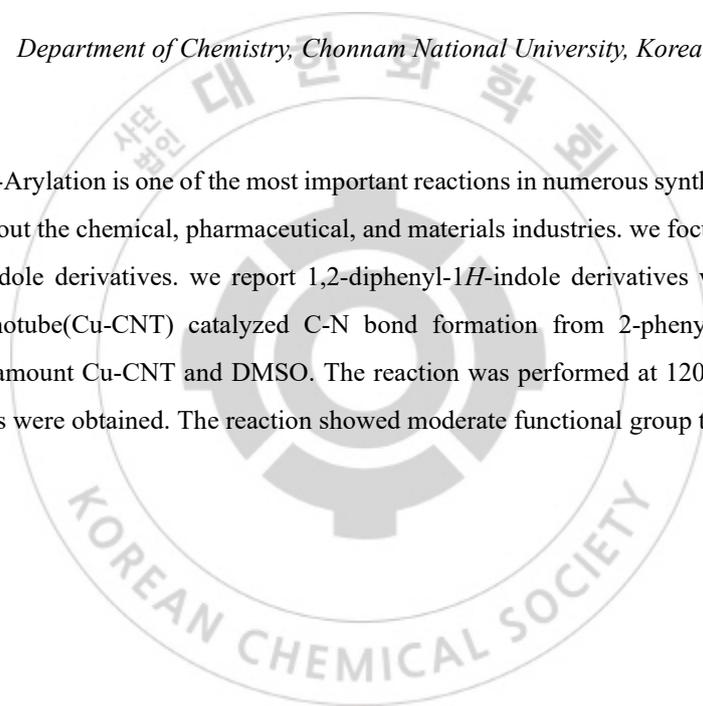
Zoom 14 FRI 15:00~16:00

Synthesis of 1,2-diphenyl-1*H*-indole derivatives by using Cu-CNT catalyzed *N*-arylation

Jeongah Lim, Sunwoo Lee*

Department of Chemistry, Chonnam National University, Korea

The formation of *N*-Arylation is one of the most important reactions in numerous synthesis of intermediates and targets throughout the chemical, pharmaceutical, and materials industries. we focus on the synthesis of 1,2-diphenyl-1*H*-indole derivatives. we report 1,2-diphenyl-1*H*-indole derivatives were synthesized via copper carbon nanotube(Cu-CNT) catalyzed C-N bond formation from 2-phenylindole, aryl halide, NaOtBu, catalytic amount Cu-CNT and DMSO. The reaction was performed at 120 °C temperature, and the desired products were obtained. The reaction showed moderate functional group tolerance.



Poster Presentation : **ORGN.P-556**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

Synthesis of β -ketoester through cross coupling of amide and ester

Joseph Devaneyan, Sunwoo Lee^{1,*}

Chemistry, Chonnam National University, Korea

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

Activated primary, secondary, and tertiary amides were coupled with enolizable esters in the presence of LiHMDS to obtain good yields of β -ketoesters at room temperature. Notably, this protocol provides an efficient, mild, and high chemoselectivity method to synthesis of β -alkylketoesters using the cross-coupling between aliphatic amides and esters. Meanwhile, gram-scale secondary and primary amides reacted via in situ generated activated tertiary amides and exhibited good reactivity when coupled with esters.



Poster Presentation : **ORGN.P-557**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

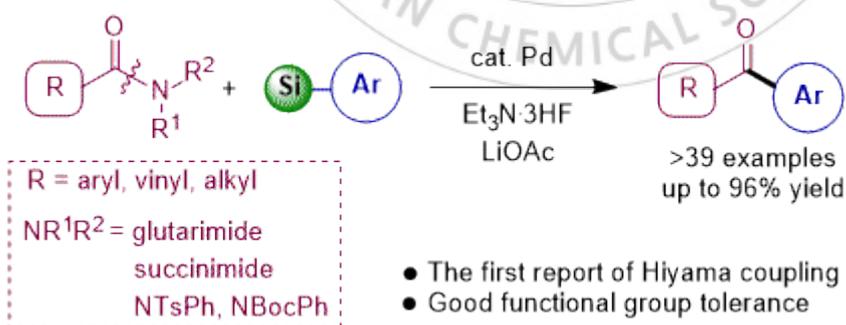
Palladium-Catalyzed Amide N–C Hiyama Cross-Coupling: Synthesis of Ketones

Muhammad Aliyu Idris, Sunwoo Lee^{1,*}

Chemistry, Chonnam National University, Korea

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

Recently, the use of amides as an acyl or aryl source in cross-coupling reactions, allowing for the synthetically-valuable functional group inter-conversion of the amide bond is gaining huge attention. Herein, we reported a palladium-catalyzed coupling of amides with arylsiloxanes to provide the corresponding arylketones via amide C–N bond cleavage. It was established that Pd(OAc)₂/PCy₃ showed the highest activity in the presence of Et₃N·3HF and LiOAc. The reaction featured broad functional group tolerance, with a variety of substituted N-benzoylglutarimides and N-alkylacylglutarimides providing the corresponding ketones in good yields. N-Benzoylsuccinimide and N-protected N-phenylbenzamides reacted with phenylsiloxane to give arylketone products in good yields.



Poster Presentation : **ORGN.P-558**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

Highly Atroposelective Pictet-Spengler Cyclization of N-Arylindoles

Aram Kim, Yongseok Kwon*

Department of Chemistry, Sogang University, Korea

Heterocycles containing nitrogen atoms are of interest as an important scaffold in the pharmaceutical and material science. In particular, N-heterocyclic biaryls are frequently found in bioactive natural products and their usefulness are appreciated in the field of asymmetric catalysis utilizing inherent axial chirality. While a number of asymmetric syntheses for axially chiral biaryls have been reported focusing on the C–C axial chirality, atroposelective reactions based on the C–N bond have been relatively less developed. Herein, we report chiral phosphoric acid catalyzed Pictet-Spengler reaction of N-arylindoles to control the axial chirality around the C–N bond via dynamic kinetic resolution. While N-arylindoles can undergo dynamic racemization around the stereogenic C–N bond, the cyclized product would have high enough rotational barrier with appropriate ortho-substituents. If a chiral phosphoric acid can interact with one atropisomer of the imine intermediate favorably and induce the catalytic cyclization, the control of the C–N bond can be realized. To avoid any possible stereochemical bias from substituted aldehydes, we tested the reaction with paraformaldehyde as an anhydrous formaldehyde source. It was found that the ortho-substituent having hydrogen-bond donor ability was necessary in the bottom aromatic ring to form favorable interactions with the chiral phosphoric acid. Further screening of reaction parameters led to the optimized reaction conditions which were applicable with a variety of substrates to show up to 98% e.e. In addition, when the substituted aldehydes were employed instead of paraformaldehyde, both of axial and point stereogenicity were controlled in up to 99% e.e. and 9:1 d.r.

Poster Presentation : **ORGN.P-559**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

A fluorescent nanoprobe for the detection of ATP based on the amine-functionalized AIEgen

NaHee Kim, Dokyoung Kim^{1,*}

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¹College of Medicine, Kyung Hee University, Korea

ATP (adenosine triphosphate) plays essential roles in the biological systems as an amino acid activator in protein synthesis, a key molecule in DNA/RNA synthesis. To date, various types of analytical methods have been developed for the analysis of ATP, including mass spectrophotometry and Raman scattering, but these methods showed limitations in the biological study and medical sample analysis. In this study, we reported a fluorescent nanoprobe for the detection of ATP. Fluorescence probes have recently attracted significant attention due to their intuitive signal response, simple operation process, selectivity, high sensitivity, and biocompatibility. The fluorescence sensing for ATP is an important assignment because there are several molecules with similar structures, such as AMP and ADP. Generally, ATP sensing approaches could be summarized in three categories: (i) Electrostatic interaction: positive-charged triamine has an interaction with a negative-charged triphosphate moiety. (ii) Chemical bond formation: vicinal diols in the ribose could make a chemical bond with aryl-boronic acid. (iii) pi-pi stacking interaction: adenine base could interact with the aromatic molecules. Within our study, a new fluorescent nanoprobe for the detection of ATP based on amine-functionalized AIEgen (aggregation-induced emission) has been introduced. The nanoprobe had no emission in the buffer (pH 7.4) due to the PET (photoinduced electron transfer) quenching effect of triamine moiety and gave strong fluorescence after the binding of ATP via pi-pi interaction and electrostatic interaction. The nanoprobe showed outstanding ATP sensing features such as high selectivity, high sensitivity, fast response time. Ref: N. H. Kim et al., Anal. Chim. Acta., 2021, 1152, 338269

Poster Presentation : **ORGN.P-560**

Organic Chemistry

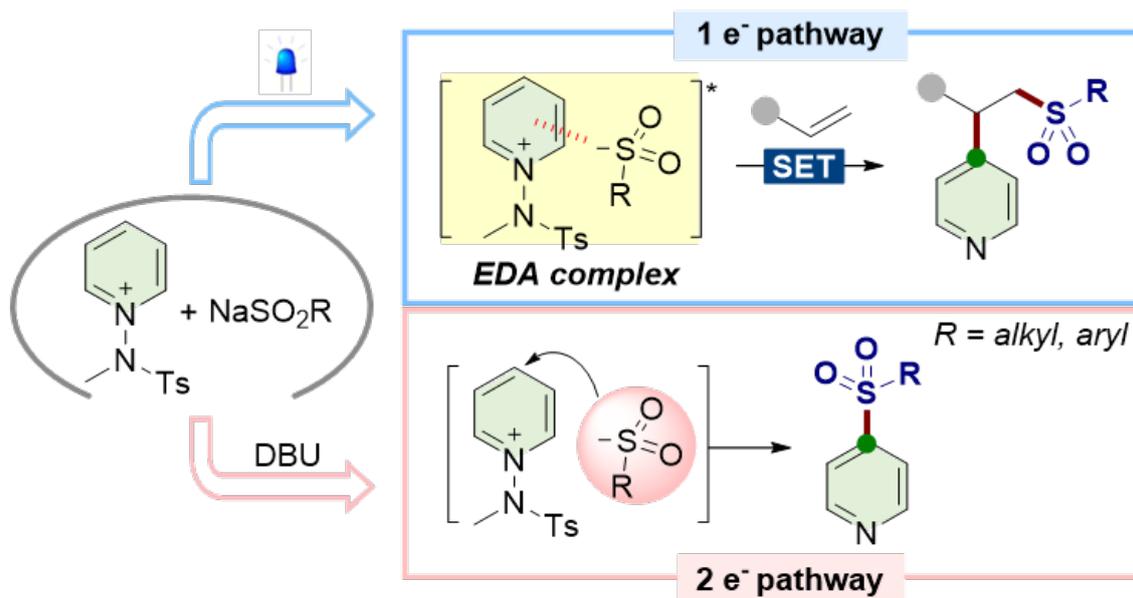
Zoom 14 FRI 15:00~16:00

Divergent reactivity of Sulfinates and Pyridinium Salts Based on One-versus Two-Electron Pathways

Myojeong Kim, Sungwoo Hong*

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

One of the main goals for modern synthesis is to develop distinct reaction pathways from identical starting materials for the efficient synthesis of diverse compounds. We disclose the unique divergent reactivity of the combination settings of pyridinium salts and sulfinates to achieve the sulfonative pyridylation of alkenes and direct C4-sulfonylation of pyridines by controlling the one- versus two-electron reaction manifolds for the selective formation of each product. Base-catalyzed coupling reaction between sulfinates and N-amidopyridinium salts led to the direct installation of a sulfonyl group to the C4 position of pyridine. Remarkably, the reactivity of this set of compounds is completely altered upon exposure to visible light: electron donor-acceptor complexes of N-amidopyridinium salts and sulfinates are formed to enable access to sulfonyl radicals. In this catalyst-free radical pathway, both sulfonyl and pyridyl groups could be incorporated into alkenes via a three-component reaction, which provides facile access to a variety of β -pyridyl alkyl sulfones. These two reactions are orthogonal and complementary, achieving a broad substrate scope and late-stage modifications under mild reaction conditions.



- *divergent reactivity by activation mode*
- *excellent functional group tolerance*
- *photocatalyst-, oxidant-free*
- *C4-selective pyridylation*



Poster Presentation : **ORGN.P-561**

Organic Chemistry

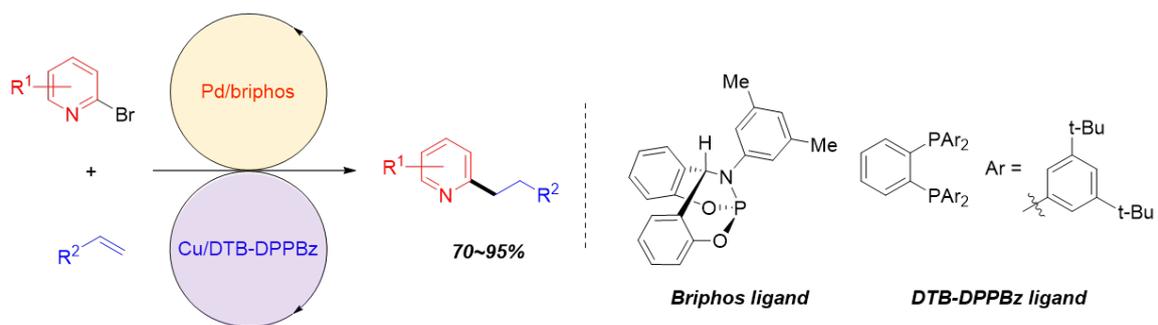
Zoom 14 FRI 15:00~16:00

Ligand Effects in Reductive C-C Cross Coupling with Electron-Deficient Aryl Bromides by Pd/Cu dual catalysts

Sanghyup Seo, Hyunwoo Kim*

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

Heterocycles are found in many organic compounds such as pharmaceuticals, agrochemicals, and natural products.¹ In order to make heteroaryl carbon-alkyl carbon bonds, Negishi or Suzuki-Miyaura cross-coupling reactions are commonly used.² However, such processes require organoboron and organozinc reagents to be prepared by multi-step reactions. In contrast, palladium and copper dual catalytic system has been developed as a complementary synthetic method for sp^2 - sp^3 cross-coupling reactions with terminal olefins and aryl bromides.³ In Pd/Cu catalyzed cross-coupling reactions, the use of electron-deficient aryl bromides still remains as a challenge. In this work, a sp^2 - sp^3 cross-coupling reaction of terminal mono-substituted olefins with electron-deficient aryl bromides has been achieved by the use of a bicyclic bridgehead phosphoramidite (briphos) ligand. This ligand is found to efficiently promote the Pd catalysis of heteroaryl bromides. Owing to strong π -acceptor ability of briphos ligand, the transmetalation and reductive elimination can be facilitated.⁴ We further investigate the use of briphos ligand for cross-coupling reactions with electron-deficient aryl bromides. **References** 1. V. F. Slagt, A. H. M. de Vries, J. G. de Vries, R. M. Kellogg, *Org. Process Res. Dev.* **2010**, *14*, 30.2. [a] K. R. Campos, A. Klapars, J. H. Waldman, P. G. Dormer, C. Chen, *J. Am. Chem. Soc.*, **2006**, *128*, 3538. [b] Y. Yang, S. L. Buchwald, *J. Am. Chem. Soc.*, **2013**, *135*, 10642. 3. S. D. Friis, M. T. Pirnot, L. N. Dupuls, S. L. Buchwald, *Angew. Chem. Int. Ed.*, **2017**, *56*, 7242. 4. [a] M. L. Clarke, M. Heydt, *Organometallics*, **2005**, *24*, 6475. [b] J. F. Hartwig, *Inorg. Chem.*, **2007**, *46*, 1936.



Poster Presentation : **ORGN.P-562**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

Synthesis of Meso Substituted Antiaromatic Hexaphyrins[1.0.1.0.1.0] (Rosarrin): Electronic Effects and Redox Properties

Chang Hee Lee^{*}, Seong-Jin Hong¹

Department of Chemistry & Biochemistry, Kangwon National University, Korea

¹Department of Chemistry, Kangwon National University, Korea

Rosarins or hexaphyrin(1.0.1.0.1.0) are unique classes of expanded porphyrinoids possessing 24 π electron system. The first synthesis of rosarin was reported in 1992 by condensation of 2,2'-bipyrrrole with benzaldehyde. This non-fluorescent rosarin is highly distorted and nonplanar geometry. Recently we have reported so called 'naphthorosarrin' having substituents either meso position or on the periphery. However, the synthesis of naphthorosarrins bearing electron donating groups at meso- position was hampered due to low yields of desired products. Here, we report the synthesis and spectroscopic and redox properties of newly synthesized naphthorosarrins bearing electron donating groups at meso-positions. Introduction of electron donating groups such as 3,5-dimethoxy and azido group, which can be readily converted to the amino group, have been synthesized. The spectroscopic studies indicates that the Solet-like band is red shifted by ~20 nm compared with rosarin containing meso-electron withdrawing groups. Upon treatment with small amount of acids, the meso-(p-aminophenyl)rosarrin is reduced to 25 π -system by one electron reduction. The electron source of this reduction is attributed to the coexisting counter anions such as chloride, bromide and iodide. These findings clearly suggest that the electron donating groups at meso-positions greatly affect on the core electronic structure and properties. Full characterization, optical properties and redox behavior of the synthesized rosarrins will be presented.

Poster Presentation : **ORGN.P-563**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

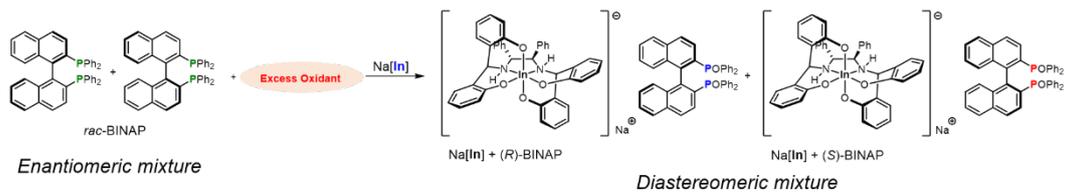
Chiral ^{31}P NMR Analysis of Phosphines and Determination of Absolute Chirality

Hyunwoo Kim^{*}, Eun Jeong Kwahk

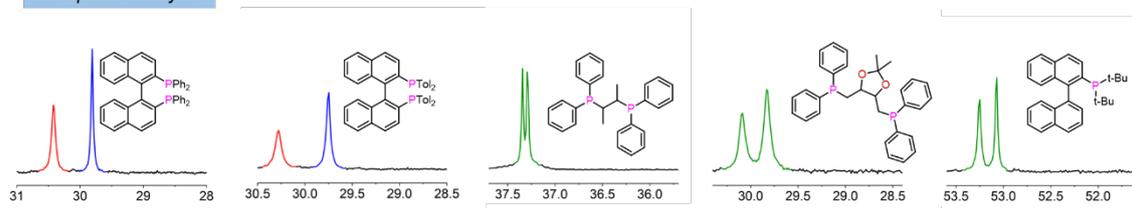
Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

Chiral phosphines are considered as privileged ligands for asymmetric reactions such as asymmetric hydrogenation, hydroformylation, and allylic alkylation with transition metals.¹ Despite the importance of chiral phosphines, methods to analyze optical purities have not been firmly established. The chiral analysis of phosphines relies on the conventional high performance liquid chromatography (HPLC) with chiral columns, or in many cases the optical purity of the phosphines was simply estimated from that of the chiral precursor owing to the lack of analytic methods. On the other hand, chiral NMR analysis is a complementary tool for determining enantiomeric excess of chiral compounds. In addition, ^{31}P NMR spectroscopy can be developed for facile chiral analysis of phosphorus-containing compounds, owing to its advantageous properties, such as no background signals and wide chemical shift range. We have previously reported that anionic chiral octahedral metal complexes can be used successfully as CSAs for chiral ^1H NMR analysis.² The substitution of Al center to Ga, Sc, and In resulted in increasing pKa values, enhancing intermolecular interactions between anionic complexes and analytes. In this work, we developed a direct chiral ^{31}P NMR analysis method that can be utilized to analyze in situ oxidized chiral phosphines by using an In complex. Baseline peak separation in ^{31}P NMR spectra was achieved for most of the chiral phosphines upon addition of In complex and oxidant. Moreover, axially chiral phosphines based on BINAP or SEGPBOS showed the same sense of peak separation, indicating the absolute chirality of phosphines. We anticipate that this chiral ^{31}P NMR analysis will be used as a universal tool to measure optical purity of chiral phosphines. References 1. Dutartre, M.; Bayardon, J.; Juge', S. *Chem. Soc. Rev.* **2016**, 45, 5771-5794. 2. Jang, S.; Kim, H. *iScience* **2019**, 19, 425-435.

Chiral ^{31}P NMR Analysis of Phosphine



Phosphine Analytes



Poster Presentation : **ORGN.P-564**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

Bipyridine containing corrole analogue and its metal complex

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The chemistry of π -extended corroles are hampered due to the synthetic challenges associated with the development of the proper 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, here we present the synthesis and spectroscopic properties of Ni(II)-complex of bipyridine containing corrole. Reaction of the free base ligand with Ni(II)(OAc)₂ resulted in the formation of anion radical of the Ni(II)-corrole complex. This esr-active complex slowly oxidized to Ni(II) neutral complex in solution over period of few days. The single electron oxidation of the anion radical of Ni(II)-corrole complex also produced a neutral Ni(II)-complex, which was fully characterized by single crystal X-ray crystallographic analysis. All the detailed synthetic, structural and spectroscopic properties of Ni(II)-complexes will be presented.

Poster Presentation : **ORGN.P-565**

Organic Chemistry

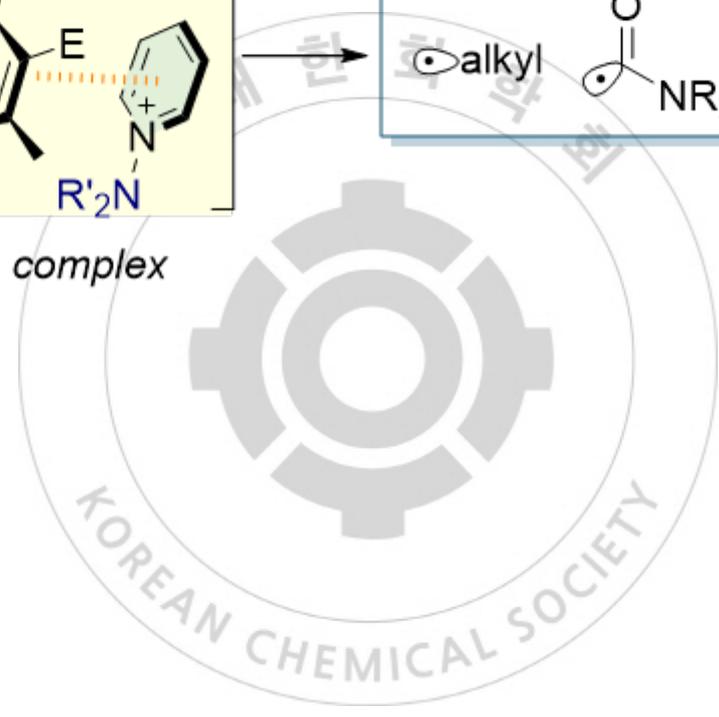
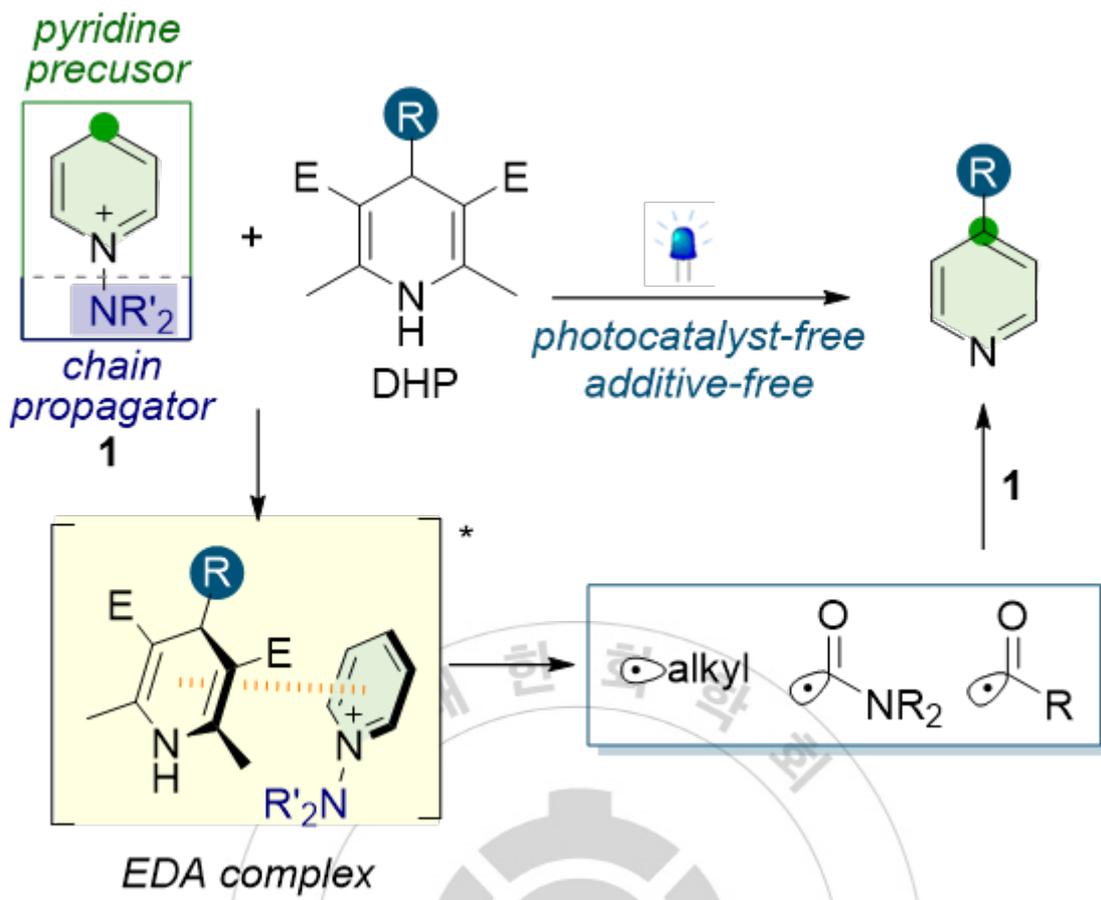
Zoom 14 FRI 15:00~16:00

Visible-Light-Enabled C4-Selective Functionalization of Pyridinium Derivatives with 1,4- Dihydropyridines

Seongjin Park, Sungwoo Hong*

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

The formation of electron donor–acceptor (EDA) complexes between 1,4-dihydropyridines and N-amidopyridinium salts under visible light irradiation enables photoinduced single-electron transfer and fragmentation to C-centered radicals without requiring a photocatalyst for the facile functionalization of pyridines. The generality of this method is demonstrated by reactions with various types of alkyl, acyl, and carbamoyl radicals derive from 1,4-dihydropyridines radical precursors, ultimately providing facile access to synthetically valuable C4-functionalized pyridines. Mild and metal-free conditions allow a broad range of functional group to be engaged in this reaction, and this is shown by the late-stage functionalization of a variety of biologically relevant pyridine-based compounds, pharmaceuticals, and peptide feedstocks.



Poster Presentation : **ORGN.P-566**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

Visible-Light Induced C(sp²)-H Amidation Involving a Skeletal Rearrangement via Redox-Neutral Radical-Polar Crossover

Hyeyun Keum, Hoimin Jung, Sukbok Chang*

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

Reported herein is the design of a redox-neutral radical-polar crossover strategy to generate selective reactivity toward radical *ipso*-addition and its applicability for the intramolecular C(sp²)-H amidation reaction, involving a skeletal rearrangement. Substrate optimization by tuning the leaving group according to the computed redox-potential led us to identify *N*-[3,5-bis(trifluoromethyl)benzoyl] group as a suitable radical precursor. *N*-benzoyloxyamide derivatives with *N*-substitution or various substituents could be broadly applied to access synthetically and pharmaceutically valuable benzofused δ -lactams by visible-light. Computational and experimental mechanistic studies were integrated to identify the origin of selective radical *ipso*-addition and subsequent C-C bond migration.

Poster Presentation : **ORGN.P-567**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

Generation and direct functionalization of α -anionic tetrahydrofuran in flow

Dongyong Kim, Hyune-Jea Lee, Heejin Kim*

Department of Chemistry, Korea University, Korea

Tetrahydrofuran (THF) is widely used as an important basic chemical feedstock and easily found as a framework in natural products and various physiological active compounds. However, the generation of α -anionic THF using a strong base such as BuLi is quite difficult due to rapid cleavage by reverse [3+2] cyclization initiated from deprotonation of α -hydrogen in THF. Herein, we reported that the generation of α -anionic THF and its serial reaction with various electrophiles was successfully achieved in flow. We fulfilled both simplicity and generality with keeping the reactivity and stability of α -anionic THF by using the flow microreactor system. The utility of α -anionic THF was expanded by successful transmetalation, both cupration, and borylation. We demonstrated that the cuprated THF chemoselectively reacted with acyl chloride in high yield. Furthermore, the continuous-flow reaction manner enabled the gram-scale synthesis of α -borylated THF in high productivity, which can be utilized for cross-coupling reaction.

Poster Presentation : **ORGN.P-568**

Organic Chemistry

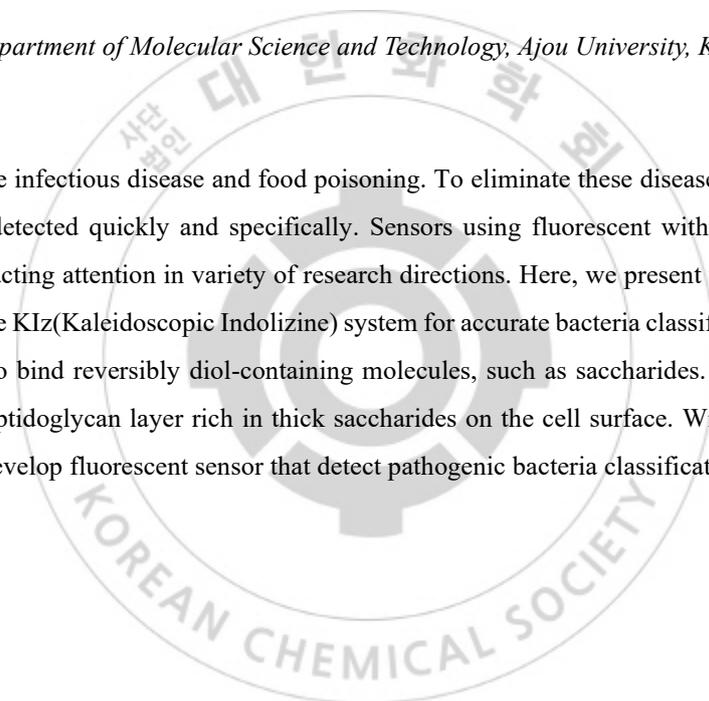
Zoom 14 FRI 15:00~16:00

Development of a fluorescent sensor based on KIz system for pathogenic bacteria

Eunha Kim^{*}, Hyungi Kim

Department of Molecular Science and Technology, Ajou University, Korea

Pathogen can cause infectious disease and food poisoning. To eliminate these diseases, pathogens such as bacteria must be detected quickly and specifically. Sensors using fluorescent with high sensitivity and selectivity are attracting attention in variety of research directions. Here, we present the development of a fluorescent with the KIz(Kaleidoscopic Indolizine) system for accurate bacteria classification. Boronic acid is widely known to bind reversibly diol-containing molecules, such as saccharides. Also, Gram-positive bacteria have a peptidoglycan layer rich in thick saccharides on the cell surface. With this approach, we successfully can develop fluorescent sensor that detect pathogenic bacteria classification.



Poster Presentation : **ORGN.P-569**

Organic Chemistry

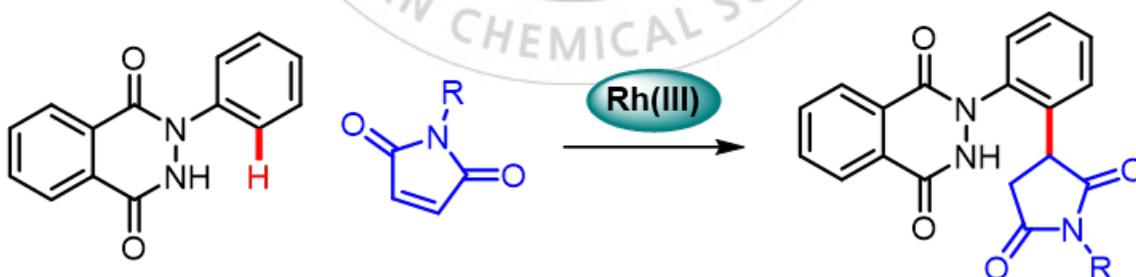
Zoom 14 FRI 15:00~16:00

Direct Combination of *N*-aryl Phthalazinone and Succinimide Moiety Using Rh(III) Catalyst

Euntaek Kim, In Su Kim*

College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea

The synthesis of *N*-Heterocycles has come to the fore in part of drug discovery and medicinal chemistry. Especially, the late-stage functionalization into bio-active moiety can supply new chance to drug discover improved pharmacological properties and physical. Phthalazinone skeleton is all around motif found in a various of pharmaceuticals, natural products, and functional materials. Particularly, this group of compounds display fascinating biological profiles such as antihypertensive, antitumor, anticonvulsant, and anti-inflammatory. In addition, succinimide scaffold is also interesting discovery in the area of medicinal chemistry. Direct combination of phthalazinone and succinimide compounds is very important to develop a synthetic method and suggest for bioactive compounds for the investigation of hit and lead candidates in drug discovery area.



Poster Presentation : **ORGN.P-570**

Organic Chemistry

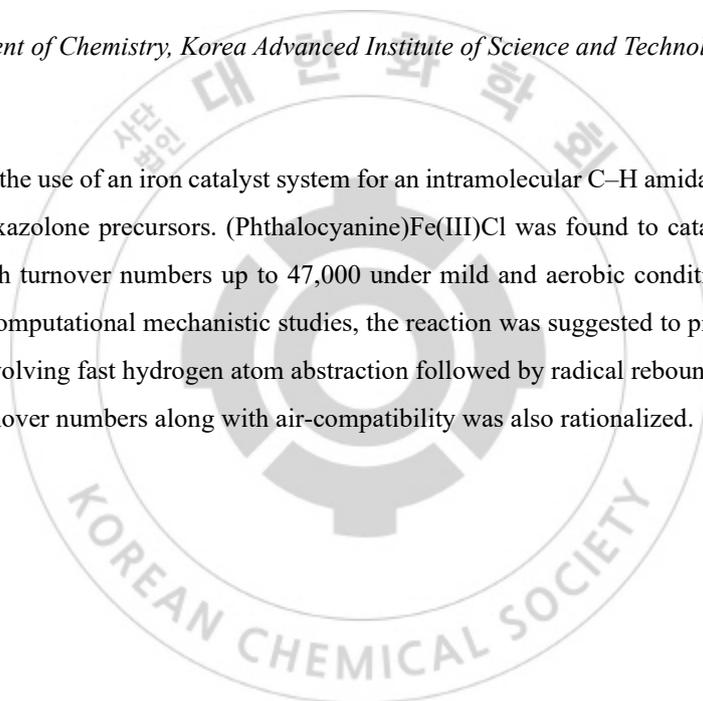
Zoom 14 FRI 15:00~16:00

Highly Robust Iron Catalyst Intramolecular C(sp³)-H Amidation Toward γ -Lactam Formation

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.



Poster Presentation : **ORGN.P-571**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

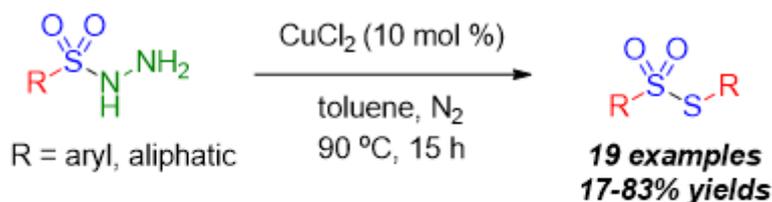
CuCl₂-promoted decomposition of sulfonyl hydrazides for the synthesis of thiosulfonates

Junsu Kim, Jinho Kim^{1,*}

chemistry, Incheon National University, Korea

¹*Department of Chemistry, Incheon National University, Korea*

Sulfonyl hydrazides recently received much attention as reagents for the introduction of sulfur-containing functional groups into organic compounds, because both sulfonyl and sulfenyl sources could be generated by the oxidation and decomposition of the sulfonyl hydrazides, respectively. However, the transformations of sulfonyl hydrazides into thiosulfonates, which could be produced by the reaction between sulfonyl and sulfenyl sources, have been less investigated. In this manuscript, we describe CuCl₂-promoted selective synthesis of thiosulfonates from sulfonyl hydrazides. A variety of thiosulfonates were produced in moderate to good yields. The mechanism involving radical intermediates such as sulfonyl radical and thiyl radical was proposed on the basis of the previously reported references and mechanistic investigations. In addition, quantum chemical simulations revealed that Cu-promoted decomposition of sulfonyl hydrazides is thermodynamically viable in the developed conditions.



- **No stoichiometric oxidant**
- **Broad substrate scope**
- **Selective and scalable**

Poster Presentation : **ORGN.P-572**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

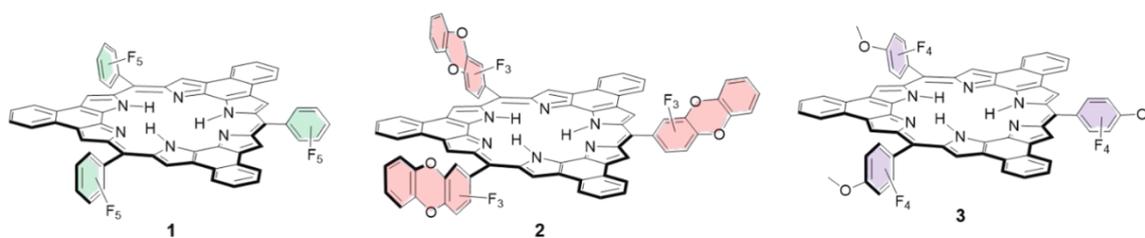
Post Synthetic Modifications of Planar Antiaromatic Hexaphyrin (1.0.1.0.1.0) by Nucleophilic Aromatic Substitution (SNAr)

Chang Hee Lee*, Ranjan Dutta¹, Seong-Jin Hong¹

Department of Chemistry & Biochemistry, Kangwon National University, Korea

¹*Department of Chemistry, Kangwon National University, Korea*

The hexaphyrin[1.0.1.0.1.0] or rosarrin (1) is a planar, fully conjugated and stable antiaromatic 24π electron system. The rosarrin 1 displayed reversible redox state changes from antiaromatic 24π electron system to aromatic 26π electron system upon protonation via proton coupled electron transfer (PCET) mechanism. In spite of this unique structural, spectroscopic and redox properties, the synthetic variants of the rosarrin 1, has been limited. Herein, we demonstrate a regio-selective nucleophilic aromatic substitution (SNAr) of meso-pentafluorophenyl group in rosarrin 1 with aromatic and aliphatic alcohols. Reaction of rosarrin 1 with catechol afforded benzodioxane fused rosarrin 2 as single product via a regio-selective, sequential SNAr. On the other hand, reaction of rosarrin 1 with methoxide (MeO-) nucleophile afforded para-OMe substituted rosarrin 3 in high yield. The synthesized rosarrins 2 and 3 exhibited noticeable changes in photophysical and redox properties compared with starting rosarrin 1. Clean, two electron reduction was achieved by treatment of both rosarrin 2 and 3 with SnCl₂•2H₂O affording the corresponding 26π -electron aromatic rosarrin analogues. Notably, significant cathodic shift in redox potentials is observed in case of rosarrin 3 which is manifested by the remarkable stability of 26π analogue. Furthermore, three state reversible switching among antiaromatic (24π), non-aromatic (25π) and aromatic (26π) analogues are demonstrated for the first time.



Poster Presentation : **ORGN.P-573**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

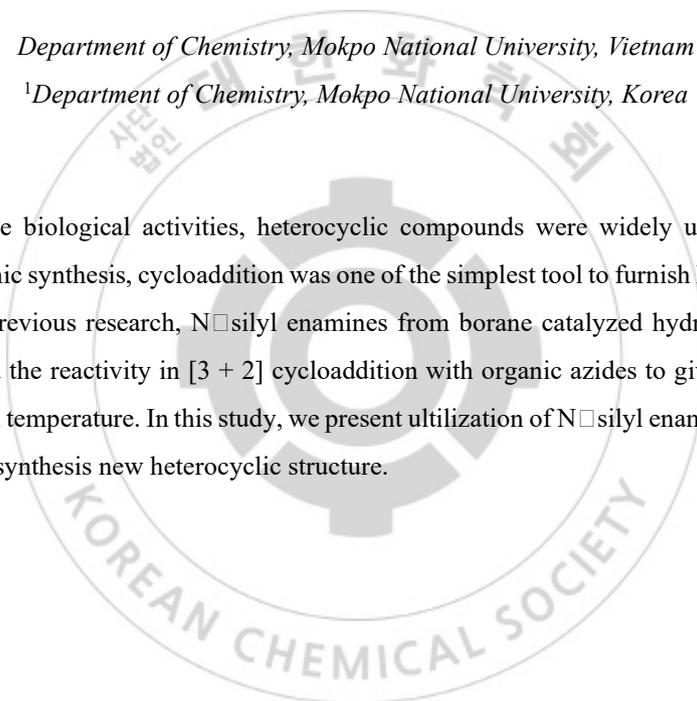
Strategy to synthesize novel heterocyclic structures from N-Silyl Enamines

Vinh Do Cao, Seewon Joung^{1,*}

Department of Chemistry, Mokpo National University, Vietnam

¹*Department of Chemistry, Mokpo National University, Korea*

Because of valuable biological activities, heterocyclic compounds were widely used in medicine and agriculture. In organic synthesis, cycloaddition was one of the simplest tool to furnish heterocyclic structure. According to our previous research, N-silyl enamines from borane catalyzed hydrosilylation of the N-heteroarene showed the reactivity in [3 + 2] cycloaddition with organic azides to give amidine with high performance at room temperature. In this study, we present utilization of N-silyl enamines as dipolarophile in cycloaddition to synthesis new heterocyclic structure.



Poster Presentation : **ORGN.P-574**

Organic Chemistry

Zoom 14 FRI 15:00~16:00

In-situ Direct ^1H NMR Chiral Analysis of Amino Acids

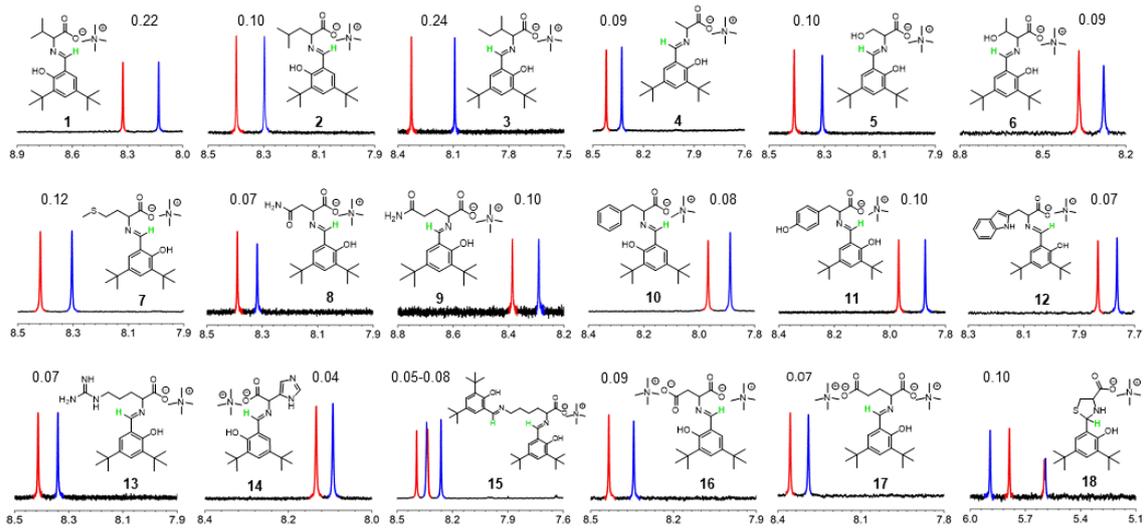
Quynh Huong Duong, Hyunwoo Kim^{1,*}

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

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

Amino acids, which are important organic molecules and serve as the building blocks of peptides and proteins, are found in wide variety of the living organisms and used as precursors in the formation of diverse chiral organic compounds.¹ However, up to now, the approaches for determination of the absolute configurations of amino acids are very limited, mainly via high-performance liquid chromatography (HPLC).² Nuclear magnetic resonance spectroscopy (NMR) has also been proven to be an operationally simple and efficient approach for chiral discrimination. Although NMR spectroscopy using a wide range of chiral solvating agents (CSAs) is commonly used to study chiral recognition with continuously expanded analyte scopes, its application for chirality assignment of amino acids still remains inadequate.³ Our research findings indicated that a chiral recognition of primary α -, β - and γ -amino acids could be proceeded via NMR using our cationic Cobalt complex as a CSA.⁴ Since the chiral analysis of α -amino acids suffered from the obvious disadvantage of their solubility in organic solvents, we treated amino acids with salicylaldehyde to form Schiff bases. Due to noncovalent interactions between CSA and the enantiomers of analyte, the diastereomeric mixture was formed. The well-resolved spectra with distinguishable peak separation of two enantiomers were obtained. The absolute configuration of amino acids was successfully determined based on the spectra of enantiopure or enantioenriched samples. We anticipate that our protocol can be a practical and useful way for the chiral analysis of α , β and γ -amino acids and their derivatives.

Reference 1. Blaskovich, MA. *J Med Chem.* **2016**, *59*(24), 10807–10836. 2. Li, X.; Cui, Y.; Xing, Y.; Lv, C.; Li, Q.; Bi, K. *Anal. Methods.* **2015**, *7*, 8817–8825. 3. Wang, W.; Xia, X.; Bian, G.; Song, L. *Chem. Commun.* **2019**, *55*, 6098–6101. 4. Jang, S.; Kim, H. *Org. Lett.* **2020**, *22*, 4185–4189.



Poster Presentation : **ORGN.P-575**

Organic Chemistry

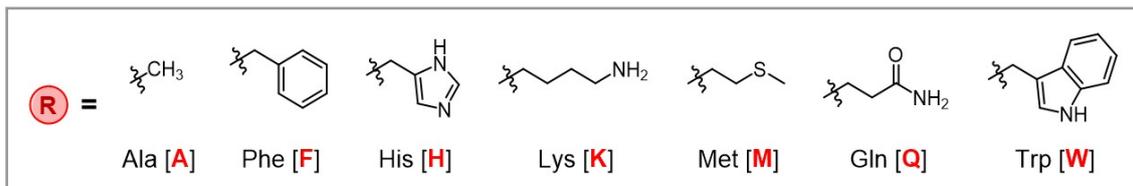
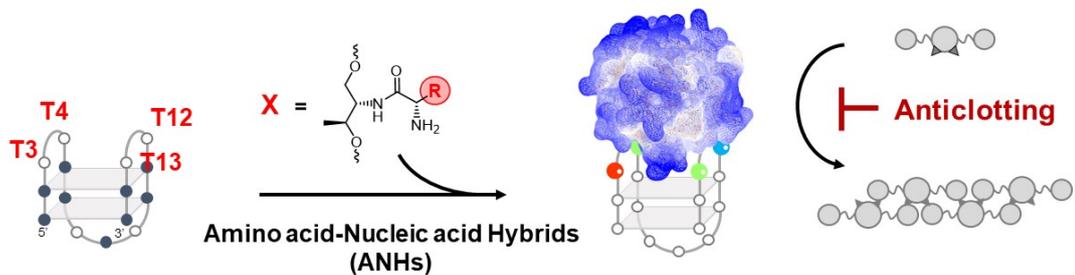
Zoom 14 FRI 16:00~17:00

Systematic DNA aptamer design with amino acid-nucleic acid hybrids (ANHs) for thrombin inhibition

Ji Hye Yum, Soyoung Park^{*}, Hiroshi Sugiyama^{*}

Graduate School of Science, Faculty of Chemistry, Kyoto University, Japan

Chemical modifications on innate DNA/RNA aptamers can significantly improve their functions. Previously, we have established a systematic modular strategy to incorporate amino acid residue into DNA oligonucleotides via an acyclic D-threoninol backbone for chemical modification of oligonucleotides. Herein, we introduce our modular strategy using amino acid-nucleic acid hybrids (ANHs) to modify a thrombin binding DNA aptamer to increase its inhibitory activity and binding affinity. (Figure 1) We chose a structurally and functionally well-defined TBA sequence (TBA15) as the basis for developing ANH-based TBA sets. A variety of ANH building blocks were incorporated instead of thymines on the loop through solid-phase DNA synthesis. All devised TBAs form antiparallel G-quadruplex structures regardless of incorporated amino acid residue. ANH-aptamers with amino acids (Phe, Met, and Trp) to replace T3 of loop region (T3F) afforded remarkably enhanced thrombin inhibition property, involving hydrophobic interaction of amino acid of modified TBA to binding site in thrombin. Moreover, surface plasmon resonance assay and molecular modeling results supports the significant difference in anticoagulation activity.



Poster Presentation : **ORGN.P-576**

Organic Chemistry

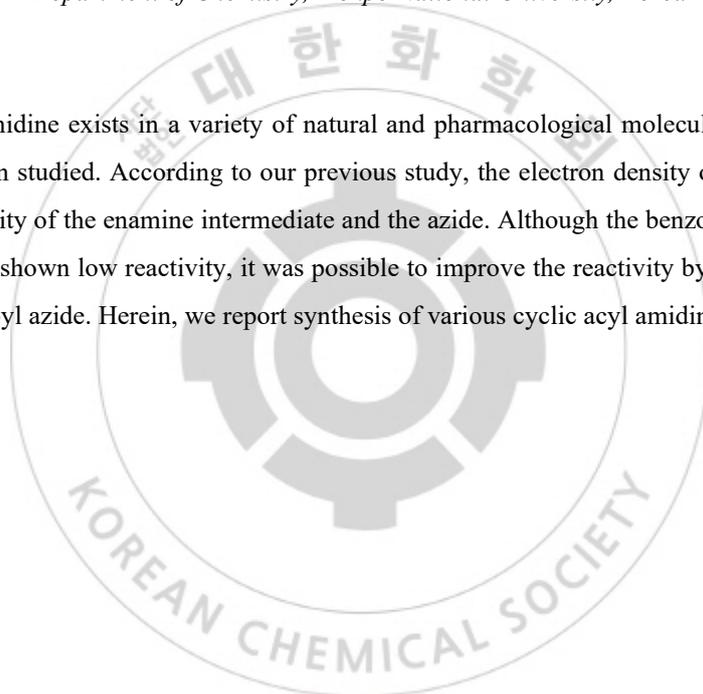
Zoom 14 FRI 16:00~17:00

Synthesis of cyclic acyl amidine from N-heteroarene and acyl azide

Dong Geun Jo, Seewon Joung*

Department of Chemistry, Mokpo National University, Korea

Since the cyclic amidine exists in a variety of natural and pharmacological molecules, various synthetic strategies have been studied. According to our previous study, the electron density of the azide critically affect to the reactivity of the enamine intermediate and the azide. Although the benzoylazide 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 acyl azides.



Poster Presentation : **ORGN.P-577**

Organic Chemistry

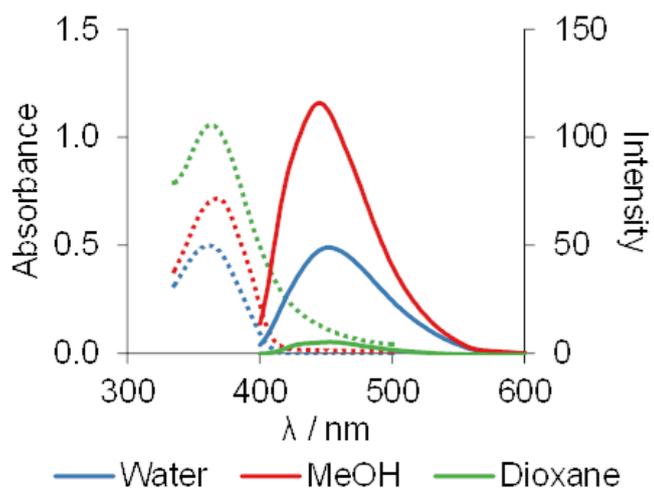
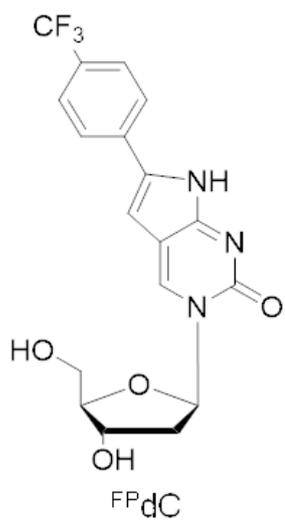
Zoom 14 FRI 16:00~17:00

Synthesis and Application of a ^{19}F -labeled Fluorescent Nucleoside as a Dual-mode Probe for i-Motif DNA Structures

Wen Ann Wee, Hiroshi Sugiyama*, Soyoung Park*

Graduate School of Science, Department of Chemistry, Kyoto University, Japan

Emissive isomorphous nucleoside analogues are versatile tools for the investigation of DNA conformations due to their stable orientations from base-pairing and stacking interactions. Furthermore, in contrast to conventional small molecules or protein dyes, emissive isomorphous nucleosides cause minimal disturbance to native DNA folding and interactions, allowing for a more accurate picture of nucleic acid structures. Herein, we report the synthesis of a fluorine-labeled fluorescent cytosine analogue, $^{\text{FP}}\text{dC}$, and its incorporation into i-motif-forming DNA sequences. DMTr-protected $^{\text{FP}}\text{dC}$ phosphoramidite was synthesized in eight steps and successfully utilized in solid-phase synthesis to obtain the desired oligonucleotides. Compared to previously reported fluorescent tricyclic cytosine derivatives, $^{\text{FP}}\text{dC}$ monomer presented a four-fold improvement in brightness (12 000) due to its high molar absorptivity ($24\ 000\ \text{mol}^{-1}\ \text{dm}^3\ \text{cm}^{-1}$) and quantum yield (0.50). When incorporated into oligonucleotides and upon formation of i-motif structures, significant changes in fluorescence intensity and lifetime, as well as ^{19}F NMR chemical shifts were observed. The changes in fluorescence intensity were observed to be highly reversible when the folding and unfolding of an i-motif structure was induced with Ag(I) ion and cysteine.



Poster Presentation : **ORGN.P-578**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

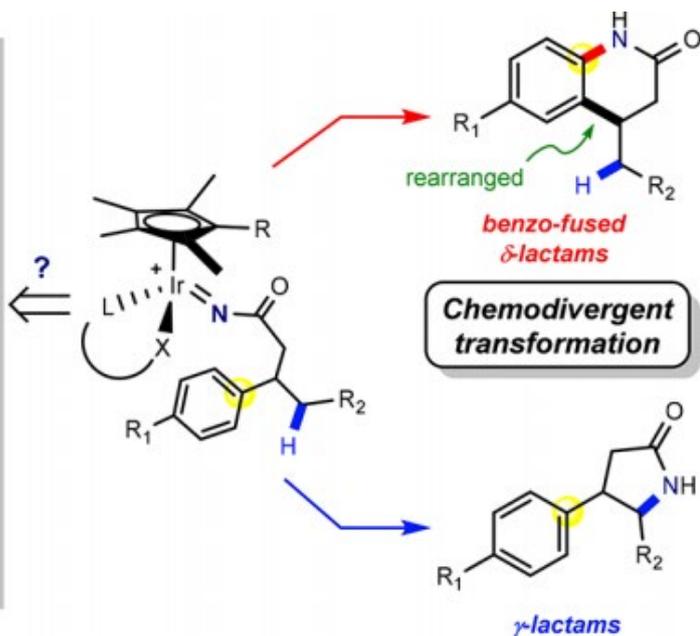
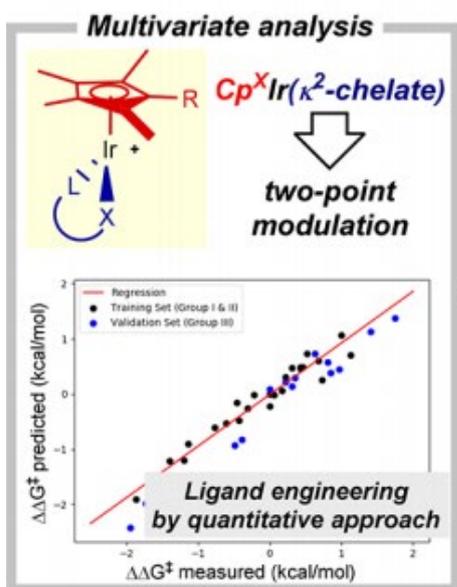
Quantitative Analysis on Two-Point Ligand Modulation of Iridium Catalysts for Chemodivergent C–H Amidation

Yeongyu Hwang, Hoimin Jung¹, Euijae Lee¹, Dongwook Kim, Sukbok Chang^{1,*}

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

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

Transition metal-catalyzed nitrenoid transfer reaction is one of the most attractive methods for installing a new C–N bond into diverse reactive units. While numerous selective aminations have been known, understanding complex structural effects of the key intermediates on the observed chemoselectivity is still elusive in most cases. Herein, we report a designing approach to enable selective nitrenoid transfer leading to sp² spirocyclization and sp³ C–H insertion by cooperative two-point modulation of ligands in the Cp^XIr(III)(κ²-chelate) catalyst system. Computational analysis led us to interrogate structural motifs that can attribute to the desired mechanistic dichotomy. Multivariate linear regression analysis on the perturbation on the η⁵-cyclopentadienyl ancillary (Cp^X) and LX coligand, wherein we prepared over than 40 new catalysts for screening, allowed for the construction of an intuitive yet robust statistical model that predicts a large set of chemoselective outcomes, implying that catalysts' structural effects play a critical role on the chemoselective nitrenoid transfer. On the basis of this quantitative analysis, a new catalytic platform is now established for the unique lactam formation, leading to the unprecedented chemoselective reactivity (up to >20:1) towards a diverse array of competing sites, such as tertiary, secondary, benzylic, allylic C–H bonds and aromatic π-system.



Poster Presentation : **ORGN.P-579**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

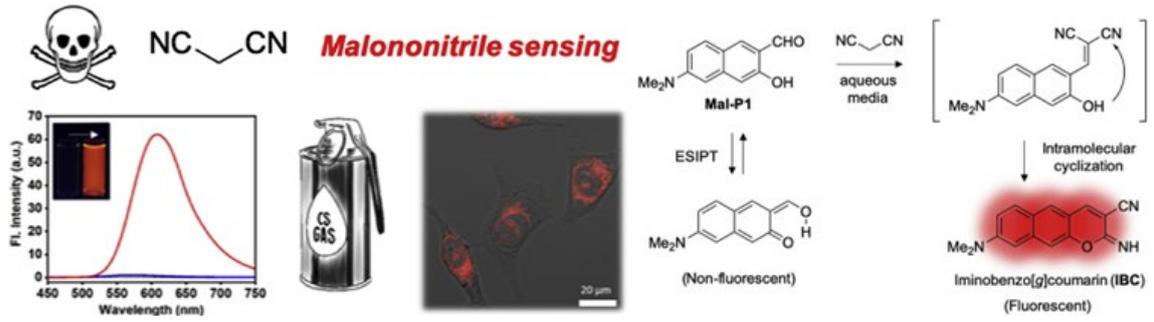
Turn-on fluorescent probe for the detection of toxic malonitrile in diverse biological and environmental condition

Yuna Jung, Dokyoung Kim^{1,*}

Department of Biomedical science, Kyung Hee University, Korea

¹*College of Medicine, Kyung Hee University, Korea*

Malonitrile ($\text{CH}_2(\text{CN})_2$), known as an active dinitrile compound, has been broadly utilized as a crucial substance in chemical synthesis, pharmaceuticals, and many industries including military use such as CS gas (tear agent; $\text{C}_{10}\text{H}_5\text{ClN}_2$; 2-chlorobenzalmalonitrile). Among them, tracing of malonitrile in the various environment (biotic, nature environment) is major because of its high toxicity. In the specific condition, malonitrile is more toxic than hydrogen cyanide (HCN), and it also associated with potential health risks and environmental pollution. In this study, we introduced a core sensing structure, 6-(dimethylamino)-3-hydroxy-2-naphthaldehyde (**MalP-1**), for the sensing of toxic malonitrile, based on the Knoevenagel condensation and intramolecular cyclization in the aqueous solvent [Ref. 1]. The malonitrile sensing abilities of **MalP-1** have evaluated by absorption/emission changes in the presence and absence of malonitrile along with varied time, concentration, and pHs. We also confirmed its selectivity and applicability on the spot by checking (i) disruption of metal ions and biomolecules, (ii) practical approach within real water, tear gas, and (iii) bio-imaging applications. In conclusion, we disclosed a new turn-on type of fluorescent probe for the detection of the toxic malonitrile, which contains great susceptibility, selectivity, and applicability. We also believe that the developed malonitrile probe holds promises on-site adaptiveness of malonitrile sensing in the healthcare, military, pharmaceutical industry, including environmental protection.[1] Y. Jung, D. Kim et al., *Anal. Chim. Acta*, 2020, 154-161.



Poster Presentation : **ORGN.P-580**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

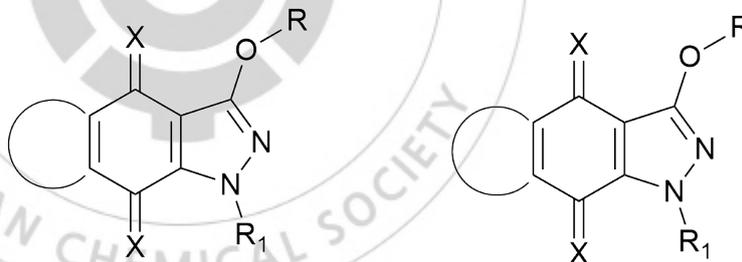
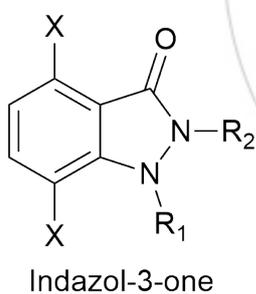
Highly Efficient Synthesis of N2-Arylindazol-3-on Derivatives.

Kyungmin Kim, Yeong Seok Kim, Heejae Choi¹, Hakwon Kim*

Department of Applied Chemistry, Kyung Hee University, Korea

¹*Applied Chemistry, Kyung Hee University, Korea*

It is very important to develop a safe, efficient and easy-to-operatable synthetic method for nitrogen-containing heterocycles. Among them, indazolone, which is composed of a benzene ring and a pyrazolone ring, exhibits various biological activities. In this study, we developed a highly efficient aryl substitution reaction of indazol-3-on at the N2-position by Chan-Evans-Lam (CEL) coupling.



Poster Presentation : **ORGN.P-581**

Organic Chemistry

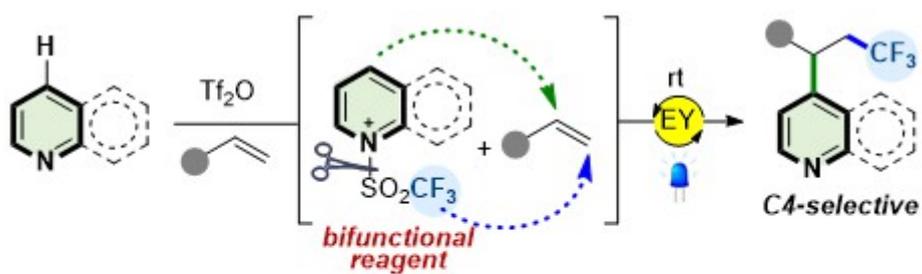
Zoom 14 FRI 16:00~17:00

Organophotocatalytic trifluoromethylative pyridylation of unactivated alkenes from simple pyridines and triflic anhydride

Kangjae Lee, Sungwoo Hong*

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

Vicinal bifunctionalization of C=C double bonds is one of important synthetic platforms to build up complex organic molecules in atom- and step-economical fashions. Especially, synchronous installation of two synthons, pyridin-4-yl and trifluoromethyl groups which are frequently seen in bioactive compounds and natural products, is considered as necessary in interdisciplinary fields including medicinal or organic chemistry. There have been several trials for alkene carbopyridylation to synthesize alkylpyridine products, but synthetic issues such as low site-selectivity and overalkylation during the pyridylation step resulted in the formation of unwanted regioisomer. Our group reported C2-selective trifluoromethylative pyridylation in intramolecular ortho-migrative manner from pyridinium salts, but C4-selective pyridylation has been remained challenging. Hence, we investigated an operationally simple and site-selective trifluoromethylative pyridin-4-ylation of unactivated alkenes. In-situ generated 1-triflylpyridinium species from pyridines and triflic anhydride serve as efficient bifunctional sources to install trifluoromethyl and pyridyl group to various alkenes accompanying the regioselective pyridylation. This synthetic strategy exhibited broad substrate scope under mild organophotocatalytic conditions, accomodating facile access to valuable C4-alkylated N-heteroarenes without the need for any pre-functionalizations on the C4 position of pyridines.



- Site-selective trifluoromethylative pyridylation
- Transition-metal free & mild photocatalytic conditions
- Broad substrate scope & late-stage functionalization



Poster Presentation : **ORGN.P-582**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

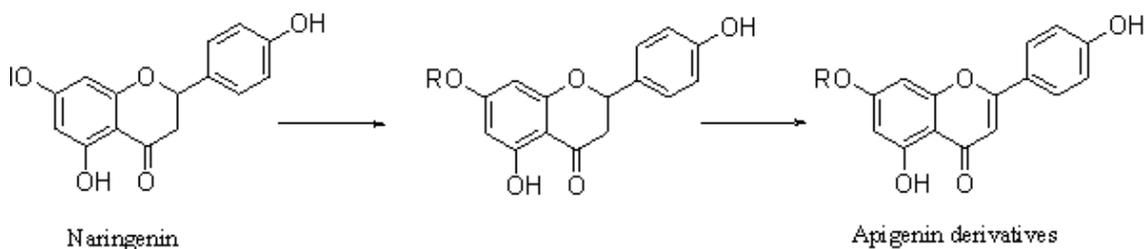
Synthesis of 7-O-alkyl or 7-O-acyl Derivatives of Naringenin and Apigenin

Mingi Chu, Dong wook Kang^{1,*}

Department of Pharmaceutical Engineering, Catholic University of Daegu, Korea, Korea

¹Department of Pharmaceutical Engineering, Daegu Catholic University, Korea

Flavonoids, known as secondary metabolites of plants and fungi, can resist allergic reactions to bacteria, viruses, and cancer, and can also prevent oxidation in the body. In addition, it is under investigation for the treatment of various diseases. When flavonoids are introduced into the body, they undergo a second relative metabolism and are present in the form of methylation, sulfation, and glucuronidation of phenolic groups, thereby showing activity. However, it is difficult to be absorbed by the gastrointestinal tract when administered orally. Therefore, it is necessary to increase the possibility of using flavonoid derivatives as disease treatment agents, so that the absorption rate and activity in the body can be improved by focusing on metabolic stability. In this study, eight derivatives that were selectively alkylated and acylated at the 7-hydroxyl group of naringenin, known as potential disease treatment candidates, were synthesized, and the synthesized derivatives were converted to apigenin to be alkylated and acylated at eight types of apigenin 7-hydroxyl groups. Then, the resulting derivatives were synthesized.



Poster Presentation : **ORGN.P-583**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

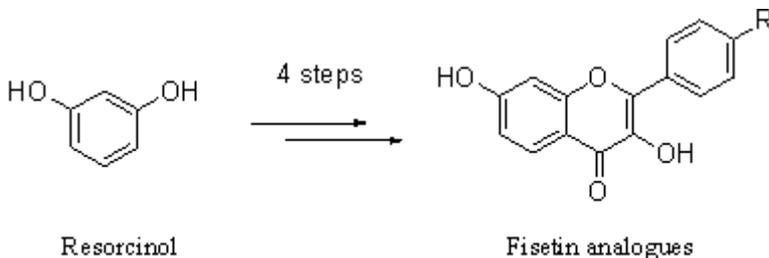
Facile Synthesis of Fisetin and Its Analogues

Mingi Chu, Dong wook Kang^{1,*}

Department of Pharmaceutical Engineering, Catholic University of Daegu, Korea, Korea

¹*Department of Pharmaceutical Engineering, Daegu Catholic University, Korea*

Flavonol-based compounds are effective in resisting reactions, such as bacteria, viruses, and allergies, and in preventing oxidation in the body. Among them, fisetin has been investigated as a therapeutic agent for various diseases, and various therapeutic effects, such as anticancer, neuroprotective, and antioxidant effects, have been confirmed. In particular, it has been reported as a potential therapeutic agent for Alzheimer's disease by inhibiting β -amyloid aggregation, which causes nerve damage, and it has been shown to improve memory by activating the signaling pathway of the hippocampus. In addition, fisetin has been reported to increase longevity, reduce aging markers in tissues, and reduce aging-related pathologies. To conduct effective research on fisetin, sufficient amount of fisetin must be secured. However, only a limited amount can be obtained through natural extraction. Therefore, it is crucial to develop an effective synthesis method for fisetin. In this study, a fisetin synthesis method that can be mass-produced through a four-step reaction from resorcinol was proposed, and two additional fisetin analogs were synthesized using this method.



Poster Presentation : **ORGN.P-584**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

Site-Selective Modification of Quinazolinones via the Rhodium(III)-catalyzed C–H Amidation of 2-Aryl Quinazolinones Using Nitrene

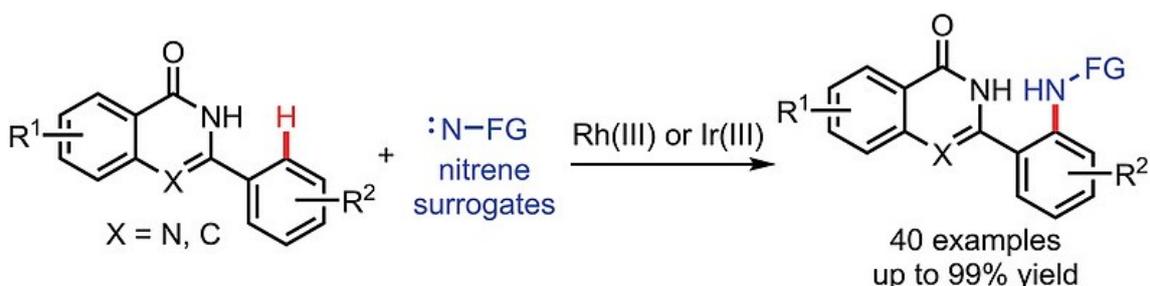
Subin Choi, Minseo Park¹, In Su Kim^{2,*}

Yuhan Corporation, Korea

¹*School of pharmacy, Sungkyunkwan University, Korea*

²*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

The carbon–nitrogen (C–N) bond is one of the fundamental bond in various pharmaceuticals and biologically relevant molecules. 2-Aryl quinazolinone motif is among the ubiquitous core found in pharmaceuticals, natural products, and advanced organic materials such as luotonin A, bouchardatin, methaqualone, and photoredox catalysts. The site-selective functionalization of quinazolinones constitute a central topic in drug discovery. In continuation of our works on the catalytic C–N bond formation reactions, we explain the Rh(III)- and Ir(III)-catalyzed C–H amidation reaction of a range of 2-aryl quinazolinones with easily accessible nitrene surrogates such as organic azides, dioxazolones, and N-methoxyamides. Especially, the late-stage C–H amidations and large-scale reaction of complex molecules demonstrate the synthetic utility of our developed method. We describe the rhodium(III)-catalyzed C–H amidation of 2-aryl quinazolinones with a range of nitrene surrogates including dioxazolones, organic azides, and N-methoxyamides. Complete site-selectivity and functional group tolerance are observed. Particularly, the large-scale reaction and late-stage functionalization highlight the synthetic potential of the developed protocol.



Poster Presentation : **ORGN.P-585**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

Merging Two Functions in a Single Rh Catalyst System: Bimodular Conjugate for Light-Induced Oxidative Coupling

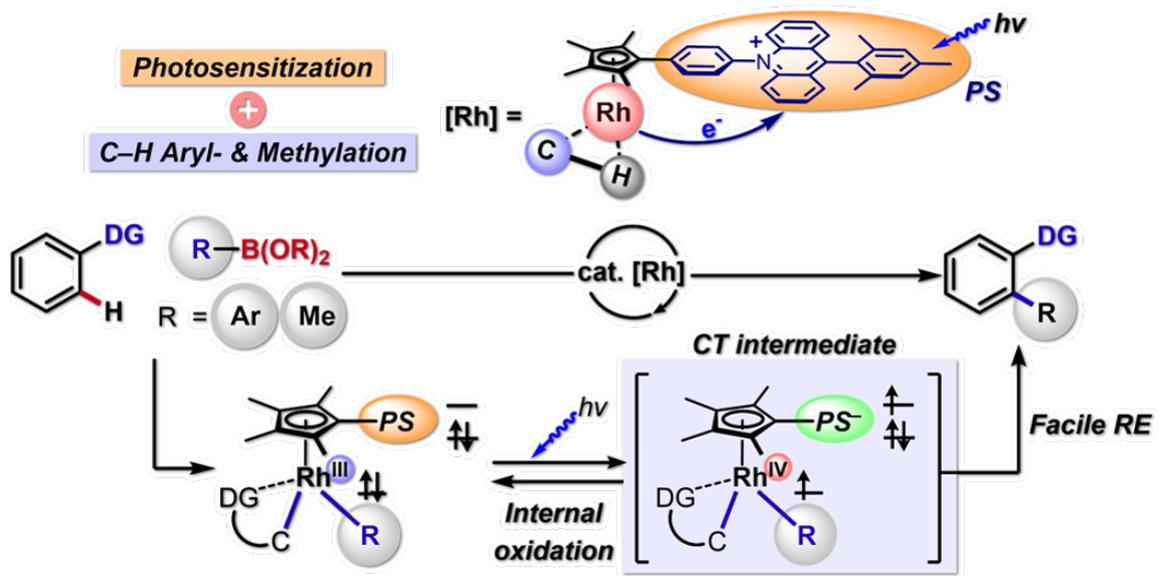
Jinwoo Kim, Dongwook Kim¹, Sukbok Chang^{2,*}

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

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²*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

In transition metal catalysis, reversible electron transfer between metal center and non-innocent ligand system has enabled versatile catalytic reactivity by tuning the metal oxidation state. In particular, light-induced metal-to-ligand charge transfer (MLCT) has paved a way to access the high oxidation state of the metal center during the catalytic process. Recent studies revealed that the formation of such transient high-valent species often significantly facilitates targeted elementary steps such as reductive elimination or ligand transfer. However, the utilization of this charge-transfer (CT) induced catalytic system on organic transformations has been underexplored, albeit its success in hydrogen transfer and CO₂ reduction chemistry. For instance, catalytic C–H transformations via CT-induced oxidative coupling have not been reported yet. In this study, we describe a single molecular, bimodular rhodium catalyst system capable of both C–H carbometalation and light sensitization, where the photosensitizer domain was designed to internally oxidize the metal center to access transient high-valent intermediate, which was confirmed by spectroscopic and electrochemical analysis. The photo-induced internal oxidation significantly facilitated the C–C bond-forming reductive elimination process from the key post-transmetalation intermediate with a notable reduction in the energy barrier, thereby enabling catalytic C–H arylation and methylation process under mild oxidative conditions.



Poster Presentation : **ORGN.P-586**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

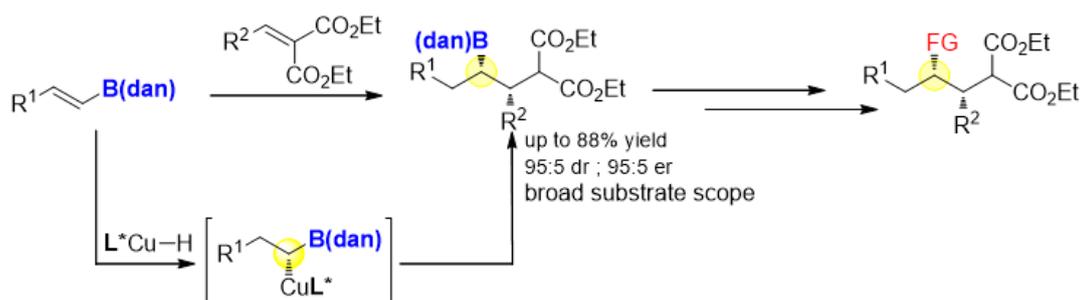
Asymmetric Copper-Catalyzed Diastereo- and Enantioselective Conjugate Addition of Alkenylboron Compounds

Jeongkyu Woo, Jaesook Yun^{1,*}

Chemistry, Sungkyunkwan University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

While important advances have been made in the asymmetric conjugate addition field, the conjugate addition with a chiral secondary alkyl metal nucleophile for the C–C bond formation has been rarely established. We report the diastereo- and enantioselective conjugate addition of chiral secondary borylalkyl copper species, in-situ generated from alkenyl boron compounds. This process produced γ -borylated diesters in good yields and high enantioselectivities up to 90% ee.



Poster Presentation : **ORGN.P-587**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

A Convenient Pinacol Coupling of Diaryl Ketones with B₂pin₂ via Pyridine Catalysis

Junhyuk Jo, Won-jin Chung*

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

With the recent prosper of radical chemistry, chemical reaction utilizing a boryl radical is studied actively.¹ The stability and persistency as well as the convenient formation method make the boryl radical useful for application to organic reactions. By taking advantage of this reactivity, we developed a pinacol coupling of diaryl ketones, which was mostly studied using reductive metals.² When a diaryl ketone is heated in the presence of diboron and pyridine, the corresponding diol is produced as a boronate form. The pyridine-boryl radical is generated via the homolytic cleavage of the pyridine-diboron complex and reacts with the diaryl ketone to give the ketyl radical. The superior reactivity of diaryl ketone was observed over monoaryl carbonyl compounds and analyzed by DFT calculation, which suggests the necessity of both aromatic rings for the maximum stabilization of the transition states.

1. a) S. Li et al., *Chem. Sci.* **2019**, *10*, 2767–2772. b) S. Li et al., *Chem. Sci.* **2018**, *9*, 3664–3671. c) L. Jiao et al., *J. Am. Chem. Soc.* **2017**, *139*, 607–610. d) X. Cheng, S. Li et al., *J. Am. Chem. Soc.* **2017**, *139*, 3904–3910. e) R. Shang, Y. Fu et al., *Org. Lett.* **2017**, *19*, 4291–4294. f) V. K. Aggarwal et al., *Science* **2017**, *357*, 283–286.

2. a) M. Szostak, D. J. Procter et al., *Chem. Rev.* **2014**, *114*, 5959–6039. b) A. Gansäuer et al., *Chem. Rev.* **2000**, *100*, 2771–2788. c) J. E. McMurry et al., *Chem. Rev.* **1989**, *89*, 1513–1524.



Poster Presentation : **ORGN.P-588**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

Fullerene C₆₀ Promoted Photochemical Hydroamination Reactions of Electron Deficient Alkyne with Trimethylsilyl Group Containing Tertiary N-Alkylbenzylamines

Hannara Jang, Dae won Cho*

Department of Chemistry, Yeungnam University, Korea

C₆₀-promoted photoaddition reactions of both trimethylsilyl- and a variety of alkyl group containing tertiary benzylamines (*i.e.*, *N*- α -trimethylsilyl-*N*-alkylbenzylamines) with dimethyl acetylenedicarboxylate (DMAD) were carried out to explore synthetic utility of trimethylsilyl group containing tertiary amines as a substrate in the photochemical hydroamination reactions with dimethyl acetylenedicarboxylate (DMAD). The results showed that photoreactions of all of trimethylsilyl containing *N*-alkylbenzylamines with DMAD, under O₂-purged environment, produced non-silyl containing enamines efficiently through a pathway involving addition of secondary amines to DMAD, former of which are produced by hydrolytic cleavage of in situ formed iminium ions. Exceptionally, five-membered N-heterocyclic rings, pyrroles, could be produced competitively in photoreaction of bulky alkyl (*i.e.*, *tert*-butyl) group substituted benzylamines through a pathway involving 1,3-dipolar cycloaddition of azomethine ylides to DMAD. Furthermore, C₆₀-sensitized photochemical reactions of non-silyl containing benzylamines with DMAD under oxygenated conditions took place less efficient and non-regioselective manner to produce enamine photoadducts. The observation made in this study show that regioselectivity of C₆₀-promoted photochemical reactions of *N*- α -trimethylsilyl-*N*-alkylbenzylamines, leading to formation of secondary amines, can be controlled by the presence of trimethylsilyl group, and that this trimethylsilyl containing tertiary amines can serve as a precursor of secondary amines for hydroamination reactions with a variety of electron deficient acetylenes

Poster Presentation : **ORGN.P-589**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

***N*-Chloro-*N*-sodio-carbamates as a Practical Amidating Reagent for Scalable and Sustainable Amidation of Aldehydes under Visible Light**

Hyunji Jeon, Wongyu Lee¹, 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*

N-Alkoxycarbonyl amides are important building blocks widely utilized in the synthesis of bioactive compounds. Despite the broad synthetic utilities, the strategies to construct *N*-alkoxycarbonyl amides are still rare, whereas those providing *N*-alkyl or *N*-aryl amides have been extensively explored. In our previous work, we reported a visible light-mediated method to convert aldehydes to amides under catalyst-, oxidant- and coupling reagent-free conditions. The applicability of this amidation was demonstrated by the late-stage functionalization, successfully proving the potentials for synthetic utility. In addition, the reaction also benefits from the low-waste-generation, not necessitating additional reagents and generating NaCl as the only waste, therefore displaying high atom-economic and sustainable chemistry credentials. Herein, we developed further improvements toward scalability and sustainability of our protocol that would provide an appealing tool for the synthesis of *N*-alkoxycarbonyl amides in industrial settings. The practicability credentials of *N*-chloro-*N*-sodio-carbamates for their use in large-scale amidation reactions are shown by scale-up productions and thermogravimetric analysis. The described amidation, which was previously hampered in sustainability perspectives by the use of α,α,α -trifluorotoluene solvent, is improved through re-optimizations using ethyl acetate as an alternative green solvent. The generality of large-scale amidations is demonstrated by the conversion of a range of aldehydes, in which the corresponding amides can be isolated in high purity without the need for special purification procedures.

Poster Presentation : **ORGN.P-590**

Organic Chemistry

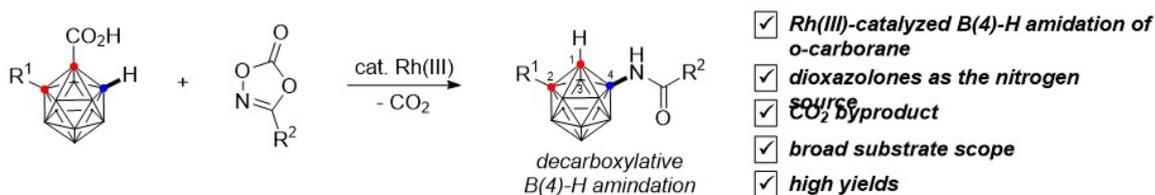
Zoom 14 FRI 16:00~17:00

Rh(III)-Catalyzed Amidation of the Cage B(4)–H Bond in *o*-Carboranes with Dioxazolones by Carboxylic Acid-Assisted B(4)–H Bond Activation

Hee Chan Noh, Kyungsup Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Because carboranes, which are a kind of three-dimensional cluster of benzene, have been increasingly investigated as boron neutron capture therapy (BNCT) agents in medicine, as versatile ligands for transition metals, and as building blocks in nanomaterials, introduction of functional groups into carborane clusters has received great attention. To date, a variety of approaches have been reported for the introduction of functional groups into CH and BH vertices of carborane clusters. Nitrogen-substituted carborane clusters have garnered significant attention over the past several years owing to their potential applications in drug and catalyst discovery. For instance, carborane clusters containing nucleoside or amino acid moieties have been used as biological active compounds for tumor treatment in BNCT. In addition, ocarborane clusters containing an aminoalkyl group have been largely utilized as ligands in organometallic chemistry. Stimulated by the recent progress in catalytic C–H amination and amidation and the distinctive function of weakly coordinating carboxylic acid as the directing group in regioselective B–H bond activation on carboranes, we have demonstrated rhodium-catalyzed direct and regioselective amidation as well as diamidation of ocarborane with dioxazolones by carboxylic acid-assisted B(4)–H bond activation in carborane clusters.



Poster Presentation : **ORGN.P-591**

Organic Chemistry

Zoom 14 FRI 16:00~17:00

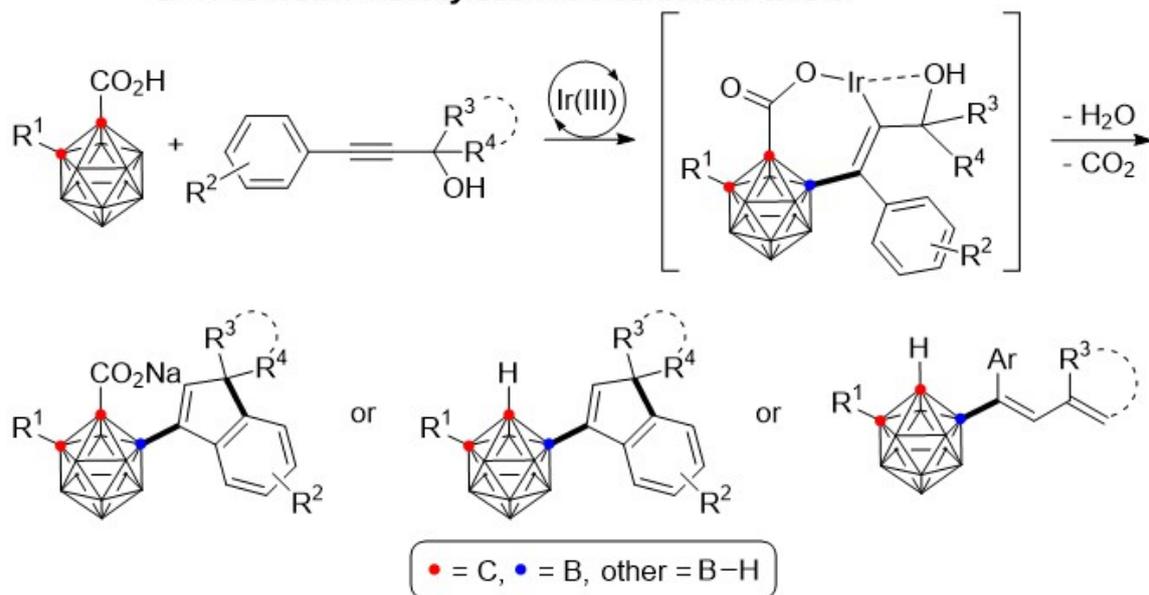
Ir(III)-Catalyzed Cyclative Indenylation and Dienylation via Sequential B(4)–C Bond Formation, Cyclization, and Elimination from *o*-Carboranes and Propargyl Alcohols

Kyungsup Lee, Eunseo Lee, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Carboranes, which are recognized as a type of threedimensional analogue of benzene, have found a variety 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 useful 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. As a result of our work, We have developed an iridium-catalyzed cyclative indenylation through B(4)–C bond formation followed by intramolecular C–C bond formation via dehydrative intramolecular electrophilic aromatic cyclization from the reaction of *o*-carborane with a variety of propargyl alcohols, affording B(4)-indenylated *o*-carboranes with excellent regioselectivity. In addition, the iridium-catalyzed regioselective 1,3-dienylation has been achieved through sequential B–H activation, dehydration, and decarboxylation, producing B(4)-dienylated *o*-carborane derivatives.

***B-H activation / Cyclative indenylation / Decarboxylation or
B-H activation / Dienylation in o-carborane cluster***



Poster Presentation : **ORGN.P-592**

Organic Chemistry

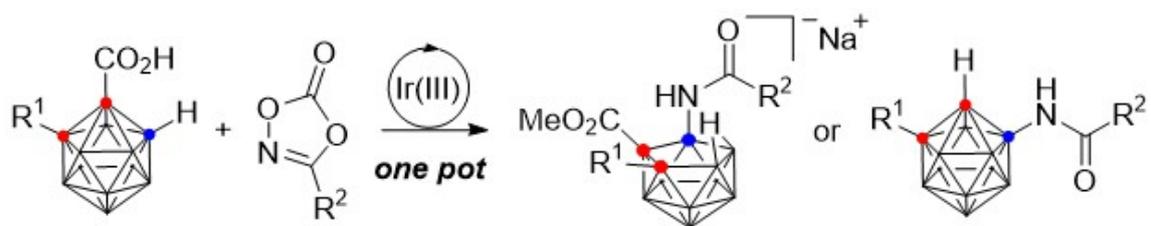
Zoom 14 FRI 16:00~17:00

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

Tae Hyeon Kim, Hee Chan Noh, 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 extremely 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 TMSCHN₂ instead of undergoing decarboxylation. Mechanism studies demonstrated that the O-methylation through trapping of acid occurred first, followed by the B(3)-deboronation.



sequential reaction in one pot trapping of carboxylic acid

nido- and closo-carboranes extremely mild conditions

= C = B other = B-H



Poster Presentation : **ORGN.P-593**

Organic Chemistry

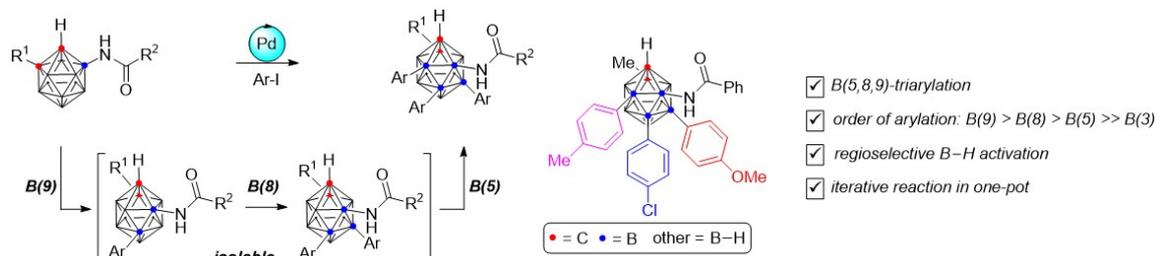
Zoom 14 FRI 16:00~17:00

Selective B(5,8,9)-Triarylation Reaction of *o*-Carboranes via Determination of the Order of Introduction of Aryl Groups into B(4)-Acylamino-*o*-carboranes

Hee Jin Yang, 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.



Poster Presentation : **ORGN.P-594**

Organic Chemistry

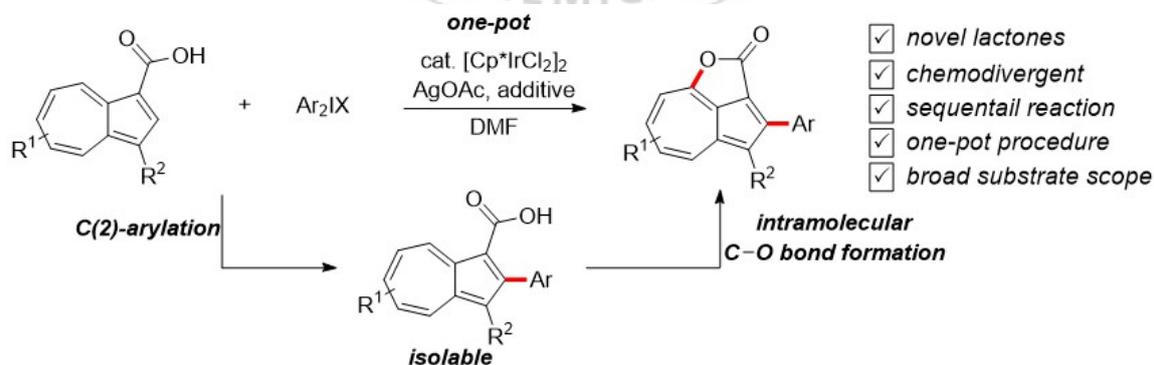
Zoom 14 FRI 16:00~17:00

Ir(III)-Catalyzed Sequential C(2)-Arylation and Intramolecular C–O Bond Formation from Azulenecarboxylic Acids and Diaryliodonium Salts Access to Azulenofuranones

Chanyoung Maeng, HanJoong Kim, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Described herein is the iridium-catalyzed sequential C(2)-arylation reaction and intramolecular C–O bond formation from azulenecarboxylic acids and diaryliodonium salts, leading to the formation of 3-arylazulenofuranones. The sequential reaction proceeded smoothly through generation of 2-arylazulene-1-carboxylic acids derived from the iridium-catalyzed regioselective C(2)-arylation reaction without the decarboxylation reaction. In conclusion, we have developed an Ir-catalyzed sequential C(2)-arylation reaction and intramolecular C–O bond formation from azulene-1-carboxylic acids and diaryliodonium salts in one pot, leading to the formation of 3-arylazulenofuranones in good yields. The sequential reaction proceeded smoothly through generation of 2-arylazulene-1-carboxylic acids derived from the iridium-catalyzed regioselective C(2)-arylation reaction without the decarboxylation reaction.



Poster Presentation : **ORGN.P-595**

Organic Chemistry

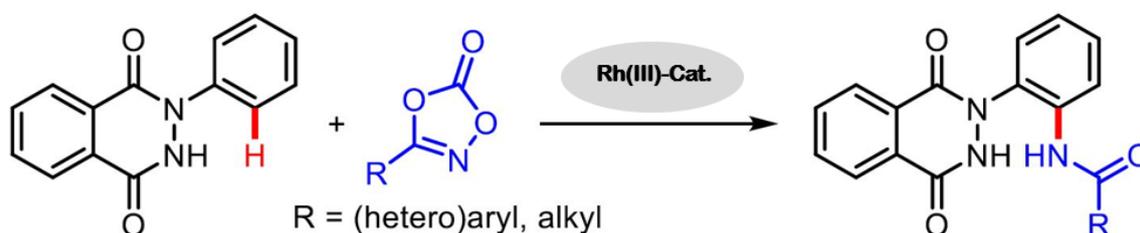
Zoom 14 FRI 16:00~17:00

Rh(III)-Catalyzed C-H Amidation of Phthalazinone Using Dioxazolones

Hyunku Ji, Suho Kim, In Su Kim*

College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea

The heterocycles containing nitrogen exist universally in nature and are closely related to heterocyclic medicinal applications. The phthalazinone skeleton is ubiquitous structural motif found in various pharmaceutical compounds such as anti-inflammatory, anti-hypertensive, anti-microbial and anti-tumors. Until now, for synthesis of the N-heterocyclic compounds, the catalytic C-H amination has been used in the most ways, and recently the new schematic method has been developed using phthalazinone derivatives under transition-metal catalysis. Even though the new protocols using phthalazinone derivatives under transition-metal catalysis developed, they have been used on the C-C bond formation using N-aryl phthalazinones and π -unsaturate substrates limitedly. By using a transition-metal catalysis such as rhodium(III) and an amide source such as dioxazolones, we propose the new protocol the C-N bond formation of N-aryl phthalazinones in the catalytic C-H amination. The new protocol can be presented a variety of applicability for the bioactive compound in drug discovery.



Poster Presentation : **ORGN.P-596**

Organic Chemistry

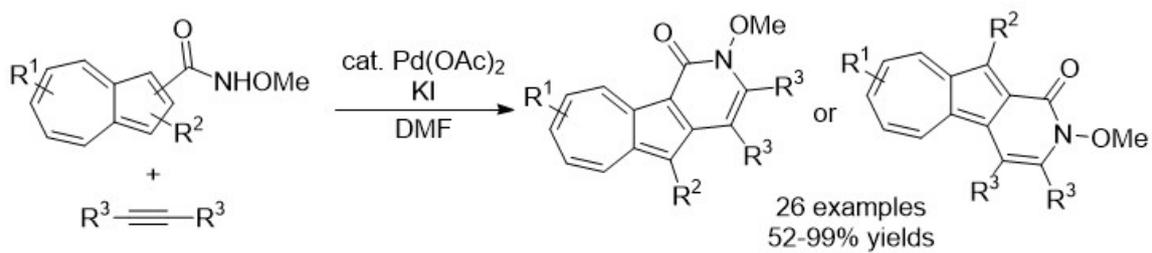
Zoom 15 FRI 15:00~16:00

Synthesis of Azulenopyridinones via Palladium-Catalyzed Oxidative [4+2] Cyclization Reactions of N-Methoxyazulene-1- and 2-carboxamides with Alkynes

Gi Uk Han, Hee Chan Noh, Phil Ho Lee*

Department of Chemistry, Kangwon National University, Korea

Azulenes, which are a class of nonbenzenoid aromatic hydrocarbons, have received prominent attention due to their importance as natural products, bioactive compounds, and molecular materials. Accordingly, the establishment of streamlined synthetic approaches for azulene skeletons from easily accessible starting materials is continuously required. Hafner and coworkers described an efficient method for azulene synthesis. However, there is a barrier to the de novo introduction of useful substituents onto the azulene ring because of the abnormal reactivity induced by the polarized π -electron system. For this reason, the functionalization of azulene through the introduction of valuable functional groups onto the preformed azulene ring and its transformation is highly attractive strategies for the synthesis of azulene derivatives. We have developed a novel synthetic method for the preparation of azulenopyridinone derivatives through a Pd-catalyzed oxidative [4 + 2] cyclization reaction of nonbenzenoid aromatic N-methoxyazulene-1- and 2-carboxamides with symmetrical as well as unsymmetrical alkynes under a molecular oxygen conditions. Broad substrate scope and excellent functional group tolerance were demonstrated. Thus, research on C-H functionalization will certainly expand to nonbenzenoid aromatic compounds in the future.



- novel skeletons*
- functionalization of azulene at 2-position*
- concise & efficient pathway*
- broad functional group tolerance*
- to overcome the natural reactivity of azulene*
- good to excellent yield*



Poster Presentation : **ORGN.P-597**

Organic Chemistry

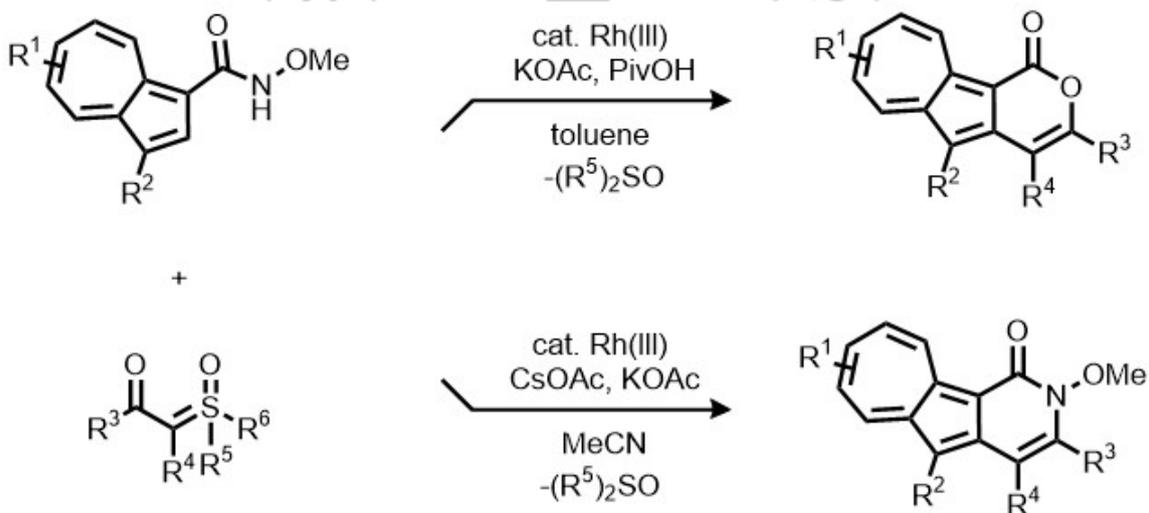
Zoom 15 FRI 15:00~16:00

Regioselective and Chemodivergent Synthesis of Azulenolactones and Azulenolactams from Rh(III)-Catalyzed Reactions of Azulenecarboxamides with Sulfoxonium Ylides

Hyeongcheol Ham, Gi Hoon Ko, 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-598**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

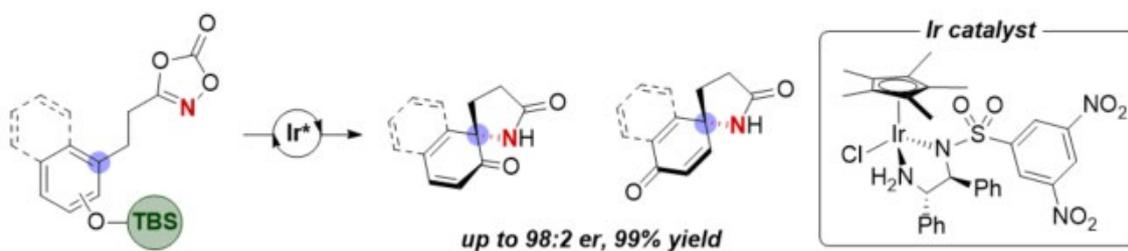
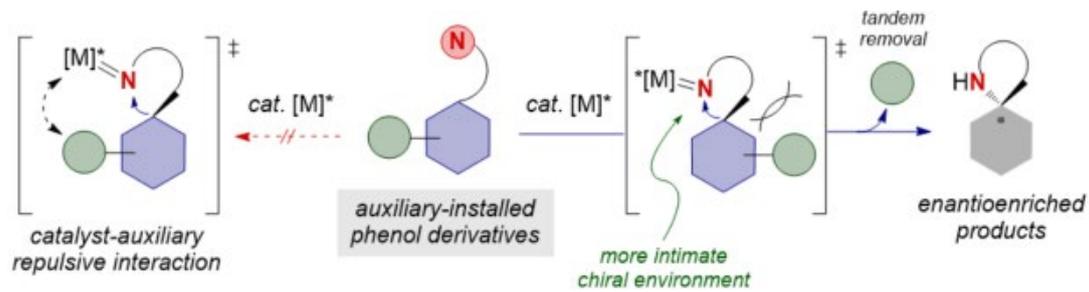
Enantioselective Access to Spirolactams via Nitrenoid Transfer Enabled by Enhanced Noncovalent Interactions

Euijae Lee, Yeongyu Hwang¹, Yeongbum Kim, Dongwook Kim¹, 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 an Ir-catalyzed enantioselective nitrenoid transfer into aromatic ipso-carbons to access chiral spirolactam products. The key strategy for precise stereocontrol was to enhance the secondary attractive and repulsive interactions in the metal nitrene addition process by installing a bulky achiral O-silyl auxiliary on phenol-type substrates, thus rendering a more intimate chiral environment by catalyst–auxiliary repulsive interactions. Moreover, upon the asymmetric spirocyclization process, the employed achiral auxiliary was expected to be removed in situ without an additional treatment. Through a well-organized chiral environment between catalyst and substrate bearing a traceless achiral auxiliary, differentiating prochiral faces of phenol-derived 1,4,2-dioxazol-5-one substrates was effectively conducted. This approach was anticipated to operate in both ortho- and para-aminative enantioselective dearomatizations to generate valuable quaternary stereocenters bearing amide functionality.



- First example of **enantioselective spiro-lactam synthesis** via Ir-nitrenoid transfer
- **Bulky O-silyl ethers** enhance the ligand-substrate secondary interactions
- Operates in both *ortho-* and *para-*dearomatizations



Poster Presentation : **ORGN.P-599**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

Ni-Catalyzed Intermolecular C(sp³)-H Amidation Tuned by Bidentate Directing Groups

Yeongbum Kim, Jeonghyo Lee¹, Jung-Woo Park², Mu-Hyun Baik^{*}, Sukbok Chang^{3,*}

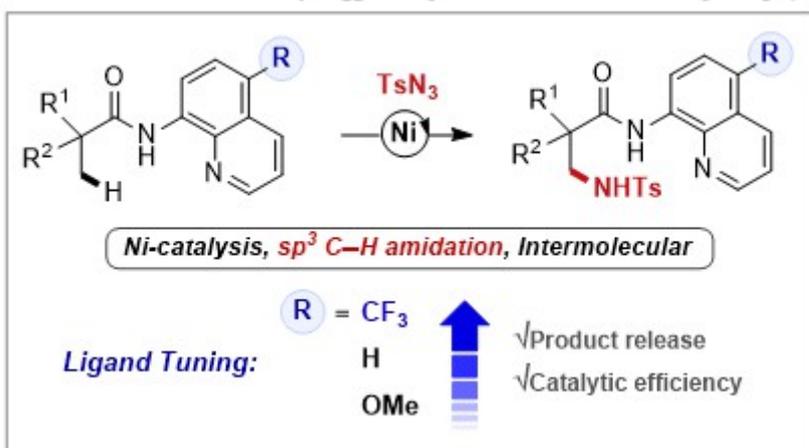
Chemistry, Korea Advanced Institute of Science and Technology, Korea

¹*Chemistry, Institute for Basic Science, Korea*

²*Department of Chemistry, Institute for Basic Science, Korea*

³*Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea*

Herein, we describe a chelation-assisted nickel-catalyzed intermolecular C(sp³)-H amidation using TsN₃ as a nitrogen source. The external oxidant-free condition enabled the selective intermolecular amidation to outcompete an intramolecular counterpart, and the electronic tuning of a directing group showed the enhanced amidation efficiency. Experimental and computational studies indicate that a putative Ni(III)-nitrenoid formed from an active Ni(II) species is involved in the present amidation reaction.



Poster Presentation : **ORGN.P-600**

Organic Chemistry

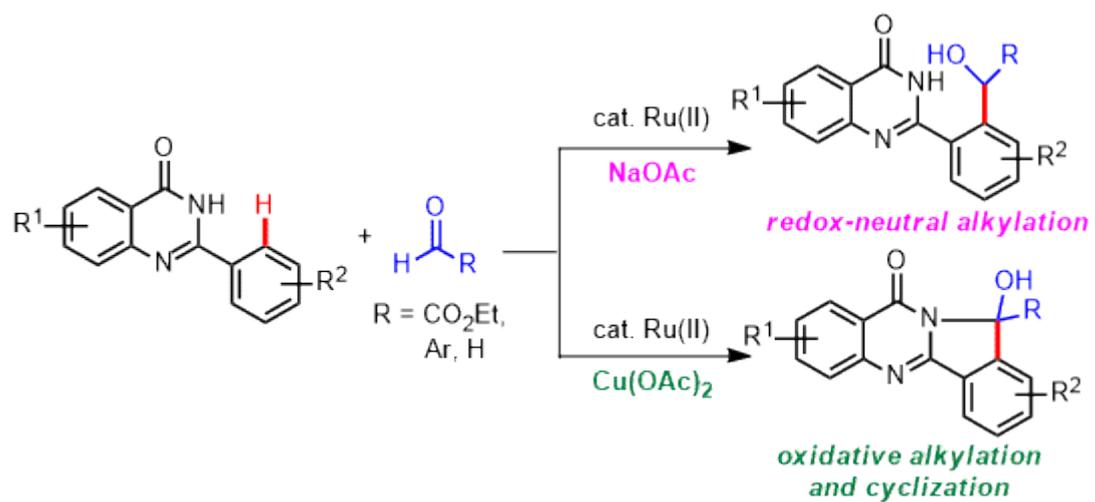
Zoom 15 FRI 15:00~16:00

C–H Hydroxyalkylation and Oxidative Cyclization of 2-ArylQuinazolinones under Ruthenium(II) Catalyst

Jin Ho Choi, Junghyea Moon, In Su Kim*

College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea

Quinazolinone skeleton is an important N-containing heterocyclic molecule which present in numerous natural products and has a range of applications in drug discovery. In particular, polycyclic quinazolinones have attracted considerable attention because of their interesting biological and physical properties. Therefore, the prevalence of polycyclic quinazolinones in bioactive molecules has led to much effort for the development of efficient methods for their preparation. In past few decades, transition-metal-catalyzed C–H functionalizations have becomes one of the most attractive area in order to the synthesis of bioactive heterocyclic molecules. In this context, much attention has been focused on the C(sp²)–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 complex as a very low-cost catalyst under mild reaction conditions. With integral structural features of unmasked 2-aryl quinazolin-4(3H)-ones with inherent directing group capability, we herein report the Ru(II)-catalyzed C–H addition and oxidative cyclization of 2-aryl quinazolinones with activated aldehydes. Notably, the employment of Cu(OAc)₂ as an external oxidant demonstrate the synthetic potential for the direct formation of polycyclic isoindoloquinazolinones. Reference1. J. H. Choi, K. Kim, H. Oh, S. Han, N. K. Mishra and I. S. Kim, *Org. Biomol. Chem.*, 2020, 18, 9611-9622.



Poster Presentation : **ORGN.P-601**

Organic Chemistry

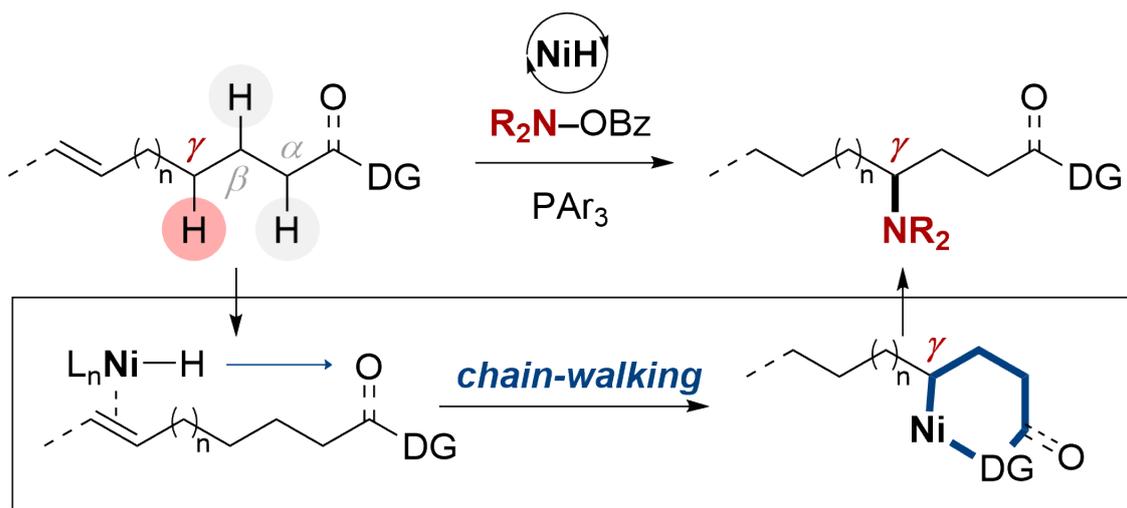
Zoom 15 FRI 15:00~16:00

Ni-Catalyzed Migratory Hydroamination: Redox Relay Strategy for γ -Selective C(sp³)-H Amination

Changseok Lee, Sungwoo Hong*

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

Migratory functionalization reactions via chain walking strategy to achieve site-selective C(sp³)-H functionalization in the presence of multiple similar aliphatic C-H bonds have attracted considerable attention. Despite the significant efforts in this field, migratory functionalization reactions are limited to C(sp³)-H α and β to polar-functional units, while γ -C(sp³)-H functionalization through controlled alkene transposition is a longstanding challenge. We reported an unprecedented γ -C(sp³)-H amination strategy of various δ,ϵ -, ϵ,ζ -, and ζ,η -alkene substrates enabled by ligand-controlled alkene isomerization and 8-aminoquinoline (AQ) directing group stabilization of the 6-membered nickellacycle, subsequently intercepted by an aminating reagents. Moreover, unusual δ -selective amination was developed by employing picolinamide (PA)-coupled alkene substrates to afford synthetically challenging and important chemical building blocks.



- remote sp^3 C-H functionalization
- excellent γ -selectivity
- broad substrate scope
- late-stage modification



Poster Presentation : **ORGN.P-602**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

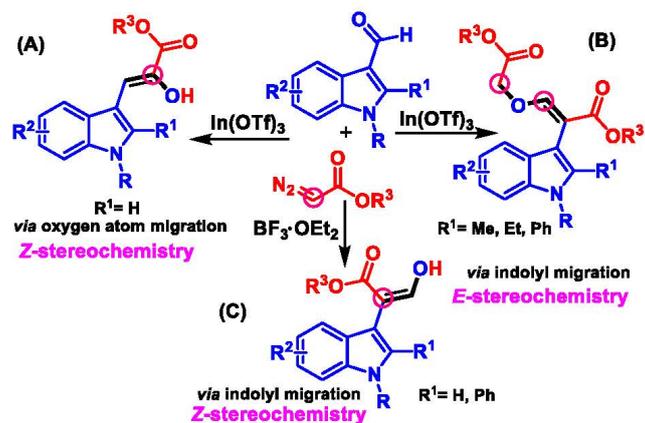
Substituent-controlled regio- and stereoselective synthesis of indolylacrylates by Lewis acid-catalyzed direct transformation of 3-formylindoles with diazo compounds

Yong Rok Lee^{*}, Sana Jamshaid¹

Division of Chemical Engineering, Yeungnam University, Korea

¹chemical engineering, Yeungnam University, Korea

An efficient and facile $\text{In}(\text{OTf})_3$ and $\text{BF}_3 \cdot \text{OEt}_2$ -catalyzed direct transformation of 3-formylindoles with diazo esters for diverse and functionalized novel indolylacrylates is developed. This one-pot protocol provides unprecedented various (Z)- α -hydroxy- β -indolylacrylates and (E)- β -(2-alkoxy-2-oxoethoxy)- α -indolylacrylates by substituent-control, regio-, and stereoselective cascade reaction. This protocol has several advantages, such as low loading of Lewis acid catalyst, mild reaction condition, broad scope, high tolerance, and higher yields. In this presentation, we report a novel and efficient strategy to synthesize biologically important (Z)- α -hydroxy- β -indolylacrylates via oxygen atom transfer (Scheme 1A), (E)- β -(2-alkoxy-2-oxoethoxy)- α -indolylacrylates via indolyl migration (Scheme 1B), and (Z)-3-hydroxy-2-indolylacrylates via indolyl migration (Scheme 1C) by $\text{In}(\text{OTf})_3$ - and $\text{BF}_3 \cdot \text{OEt}_2$ -catalyzed reactions of 3-formylindoles with diazo esters. The synthesized compounds are further converted into biologically interesting materials.



Scheme 1. New synthetic strategies for 3-Functionalized Indoles starting from 3-Formylindoles and Diazoacetates

Poster Presentation : **ORGN.P-603**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

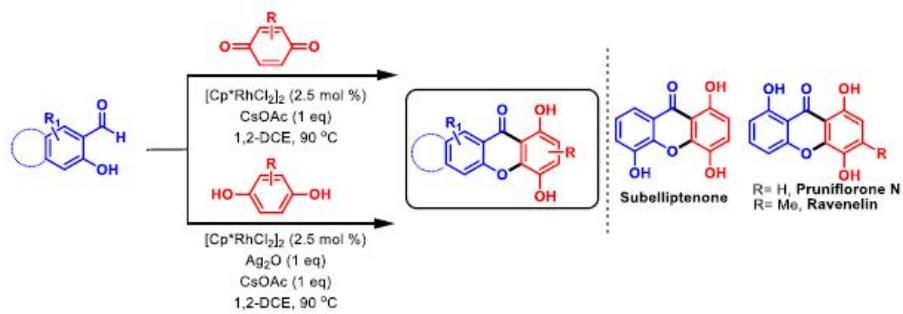
Rh-Catalyzed Double C–H/O–H Functionalization of Salicylaldehydes with 1,4-Benzoquinones or 1,4-Hydroquinones for Diverse Xanthone Frameworks

Sagar Nale, Yong Rok Lee^{1,*}

school of chemical engineering, yeungnam university, Korea

¹Division of Chemical Engineering, Yeungnam University, Korea

Xanthenes are privileged oxygen-containing heterocycles found widely in synthetic and natural products. In particular, multihydroxylated xanthenes bearing 1,4-dihydroxyl groups have shown potent anticancer, antidiabetic, antiplasmodial, antimicrobial, and anti-inflammatory activities. Owing to their importance, several exciting synthetic procedures for xanthone skeletons including biosynthetic approaches have been reported. Although several contributions have been demonstrated in recent years, there is no report on the synthesis of divergent and polyfunctionalized xanthenes by transition-metal-catalysed aldehydic C–H activation of salicylaldehydes with readily available 1,4-benzoquinones or 1,4-hydroquinones. This work represents the first example on direct construction of polyhydroxylated xanthenes bearing polyols, chiral moieties, polycyclic rings, and polyaromatic rings by Rh-catalyzed double C–H/O–H functionalization of salicylaldehydes with 1,4-benzoquinones or 1,4-hydroquinones (Scheme 1). This protocol can be further extended to obtain biologically active materials through late-stage functionalization, and affords natural products such as subelliptenone, pruniflorone N, and ravenelin in a single step.



Scheme 1. Rhodium(III) Catalyzed Double C–H/O–H Functionalization for Diverse Xanthenes.



Poster Presentation : **ORGN.P-604**

Organic Chemistry

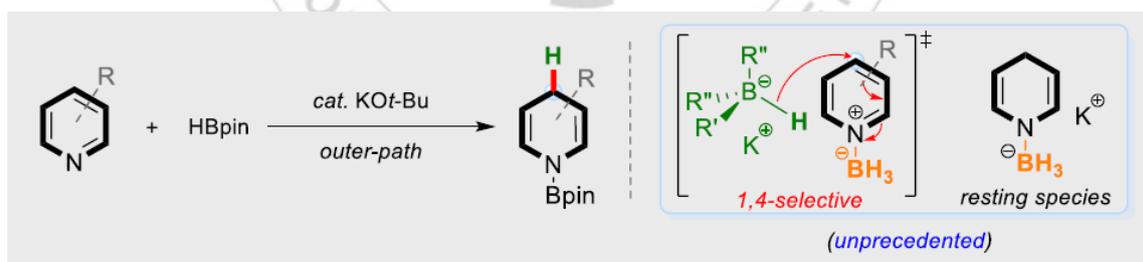
Zoom 15 FRI 15:00~16:00

Alkoxide-Promoted Selective Hydroboration of N-Heteroarenes: Pivotal Roles of in situ Generated BH₃ 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 document-ed 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-BH₃ adducts undergo a hydride attack by alkoxyborohydrides, (ii) in situ generated BH₃ serves as a catalytic promoter, and (iii) 1,4-dihydropyridyl borohydride is in a predominant resting state.



Poster Presentation : **ORGN.P-605**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

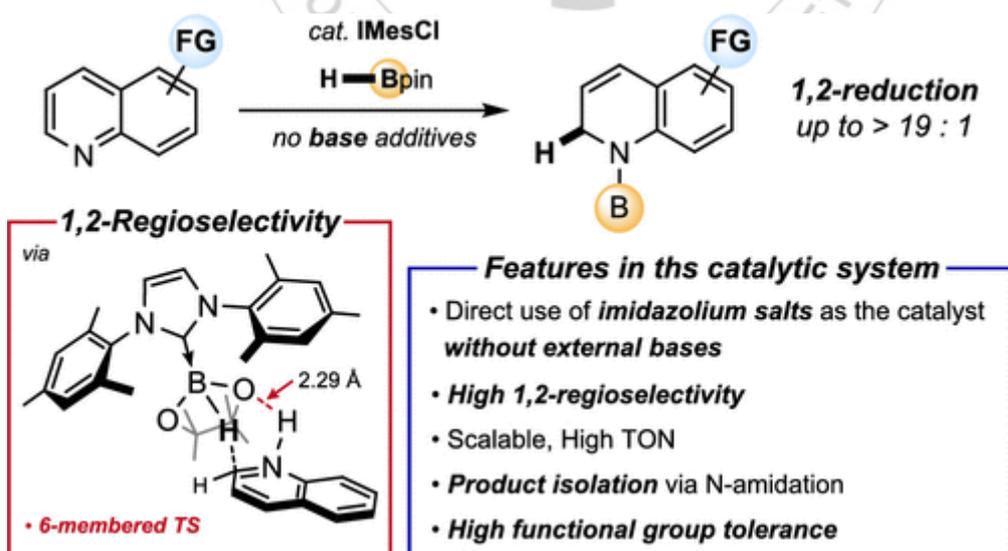
NHC-Catalyzed 1,2-Selective Hydroboration of Quinolines

Joon Heo, Dongwook Kim¹, Sukbok Chang^{*}

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

¹*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

Selective dearomative transformation of readily available N-heteroarenes is a powerful tool accessing useful synthetic building units. Described herein is the NHC-catalyzed 1,2-selective hydroboration of quinolines with high functional group tolerance. Dihydroquinoline products could be isolated as their amide derivatives upon in situ N-protection, thus offering high synthetic utility of the current procedure. Combined experimental and computational studies revealed that the observed regioselectivity can be rationalized by proposing a six-membered transition state that collectively incorporates NHC catalyst, hydroborane reductant, and protonated quinoline substrate.



Poster Presentation : **ORGN.P-606**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

Cobalt-Catalyzed Intermolecular C–H Amidation of Unactivated Alkanes

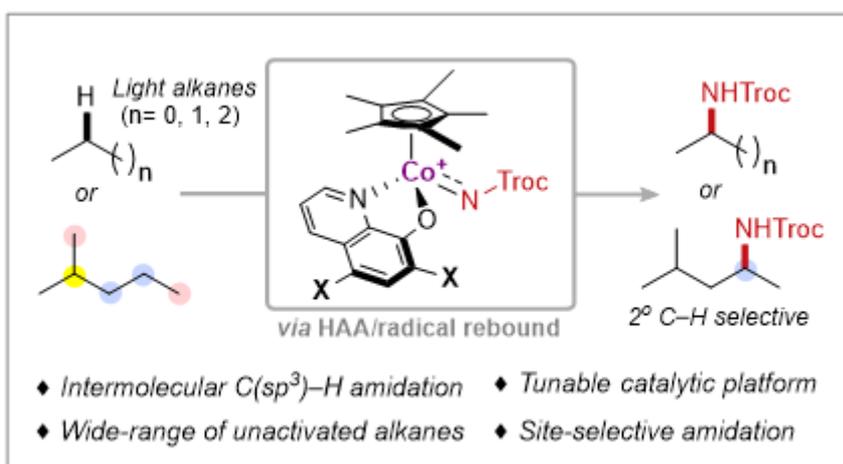
Jeonghyo Lee, Seongho Jin¹, Dongwook Kim², Soon Hyeok Hong^{1,*}, Sukbok Chang^{1,*}

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*

Alkanes are an abundant and inexpensive source of hydrocarbons, thus development of new methods to convert the hydrocarbon feedstocks to value-added chemicals is of high interest. However, it is challenging to achieve such transformation in direct and selective manner mainly due to the intrinsic inertness of their C–H bonds. We herein report a tailored Cp*Co(III)(LX)-catalyzed efficient and site-selective intermolecular amidation of unactivated hydrocarbons including light alkanes. Electronic modulation of the cobalt complexes led to the enhanced amidation efficiency, and these effects were theoretically rationalized by the FMO analysis of presupposed cobalt–nitrenoid species. Under the current cobalt protocol, a secondary C–H bond selectivity was observed in various nonactivated alkanes to reverse the intrinsic tertiary preference, which is attributed to the steric demands of the cobalt system that imposes difficulties in accessing tertiary C–H bonds. Experimental and computational studies suggested that the putative triplet Co-nitrenoids are transferred to the C–H bonds of alkanes via a radical-like hydrogen abstraction pathway.



Poster Presentation : **ORGN.P-607**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

Facile Synthesis of Highly Functionalized Xanthene Fluorophores via Indium-Catalyzed Cascade Reaction

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chemical engineering, Yeungnam University, Korea

¹*Division of Chemical Engineering, Yeungnam University, Korea*

The xanthene motif is an important structural entity found in numerous biologically interesting natural and synthetic products. They exhibit diverse pharmaceutical activities and are used for photodynamic therapy and cell imaging. The xanthene motif is also utilized as a building block for the synthesis of bioactive molecules and functional materials. Although several methods for the synthesis of xanthenes and their functionalization have been well demonstrated, more straightforward and efficient synthetic approaches are still required. Till date, no study has yet investigated the formation of xanthenes bearing the biologically interesting oxindole moiety using Lewis acid-catalyzed cascade reactions between 1,4-benzoquinones and oxindoles. In this presentation, this work describes a facile and efficient protocol for the synthesis of various xanthenes bearing biologically interesting oxindole nucleus by In(III)-catalyzed reactions of quinones and oxindoles. This novel reaction proceeds via cascade double Michael-additions and intramolecular cyclization. The synthesized compounds exhibit the possibility of use as a new fluorophore for selective imaging sensing of heavy metal in living cells.

Poster Presentation : **ORGN.P-608**

Organic Chemistry

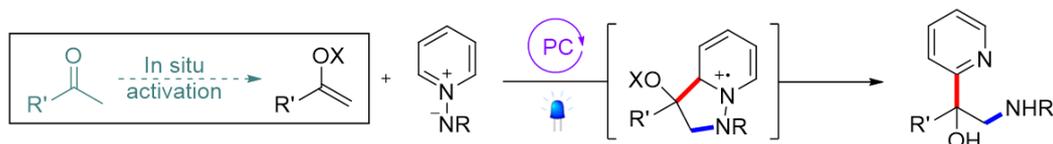
Zoom 15 FRI 15:00~16:00

A Double Umpolung Strategy using Photocatalysis for the Vicinal Aminopyridylation of Methyl Ketones

Wonjun Choi, Sungwoo Hong*

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

Photocatalytic vicinal aminopyridylation of methyl ketones by double umpolung strategy is enabled using *N-N* ylides. Polarity inverted products are synthesized by radical mediated 1,3-dipolar cycloadditions with enolsilanes activated in situ from methyl ketones and single electron oxidized *N-N* ylides by photocatalysis, followed by *N-N* bond homolytic cleavage. Unusually, electrophilic carbonyl carbon and nucleophilic α -position are bond with electrophilic C2 position of pyridyl group and nucleophilic amidyl group respectively that can not access by their innate polarity. A broad scope and late-stage functionalization of complex molecules are showed utility of this method. Also this strategy can be applied to enamides in stead of enolsilanes.



Poster Presentation : **ORGN.P-609**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

Water-mediated Photocatalytic Membrane Oxidation in Hypoxic Cancer Cells

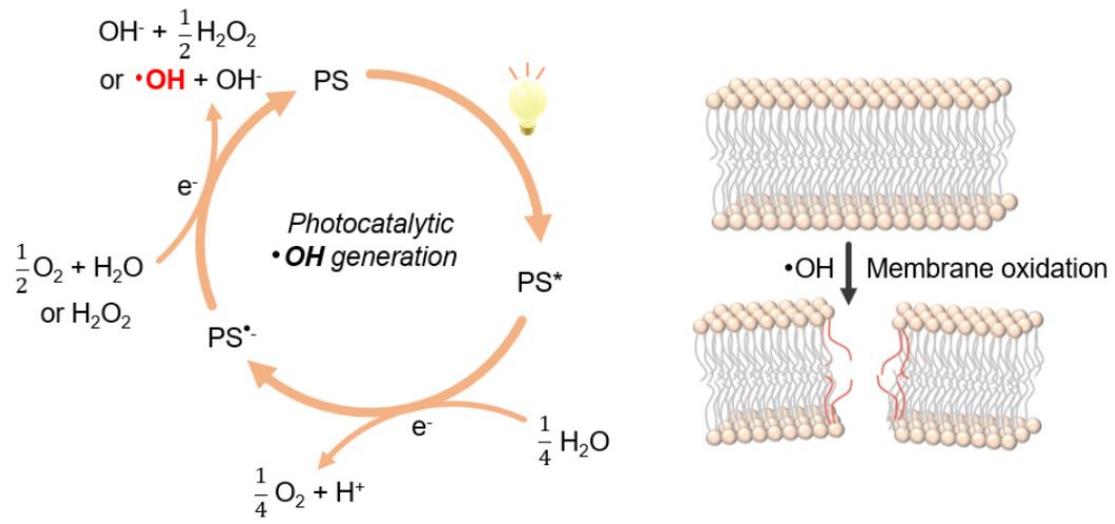
Chaiheon Lee, Mingyu Park¹, Tae-Hyuk Kwon^{2,*}

Chemistry, Ulsan National Institute of Science and Technology, Korea

¹*Ulsan National Institute of Science and Technology, Korea*

²*Department of Chemistry, Ulsan National Institute of Science and Technology, Korea*

A hypoxic tumor environment driven by aggressive cellular proliferation and abnormal vascularization has been a severe challenge to treating solid tumors. Under hypoxia, cancer cells with insufficient nutrients operate the self-protection process to survive by altering their metabolism, protein composition, and gene expression. These alterations trigger acceleration of the DNA repair process, inhibition of apoptosis, increased drug efflux, and decreased drug influx, leading to resistance to chemotherapy, then cause the failure of cancer therapy. Photosensitizers for photodynamic therapy (PDT) have been considered promising therapeutics. Photosensitizers show therapeutic features to cancer cells with chemoresistance because photosensitizers cause severe oxidative stress to antiapoptotic proteins, drug-efflux pumps, and membranes. However, the activation of photosensitizer is highly dependent on the cellular oxygen level. Therefore, for the hypoxic cancer cells, traditional PDT represents diminished treatment efficiency even though PDT does not cause cross-resistance to chemo- and radiation therapy. In this work, we synthesized a membrane-localized donor-acceptor (D-A) type photosensitizer producing hydroxyl radical from water molecules. This photosensitizer strongly oxidizes unsaturated lipids and membrane proteins to disrupt the cellular membrane, leading to cell death under hypoxic conditions. In addition, the cell death is independent of the apoptotic pathway, which implies the water-mediated photocatalytic membrane oxidation has the potential to treat the hypoxic tumor.



Poster Presentation : **ORGN.P-610**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

A lysosome localized iridium complex inhibits autophagy by impairing membrane lipids and oxidizing membrane constitution and fusion related proteins.

Mingyu Park, Jung Seung Nam, Tae-Hyuk Kwon*

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

Lysosome has currently been highlighted for its crucial roles in intracellular communication. Its controlled dysfunction may lead to fatal damage on a cancer cell. However, a precise mechanism after lysosomal damage has not yet been perfectly understood. This research aims to elucidate the start-to-end cell death pathway using lysosome localized reactive oxygen species (ROS) generation. Newly designed organometallic iridium (ii) complexes, B2 and B4, were used for the specific lysosomal oxidative stress. Analyses on oxidative residues, microscopic images, immuno staining results, and oxidized protein network indicated that the iridium complexes impair autophagic flux by lysosomal membrane permeabilization, membrane sustainment related protein oxidation, and membrane fusion responsible protein oxidation. This study is expected to feature the effectiveness of lysosome target ability.

Poster Presentation : **ORGN.P-611**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

A ratiometric fluorescent sensor based on γ -cyclodextrin inclusion complexes of self-assembled pyrenyl-nanofibrils for quantitative detection of α -amylase activity

Tae Min Park, Seung Yeob Lee, Su Jin Na, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

In this work, an effective fluorescent biosensor have been developed for quantitative detection of α -amylase activity on the basis of inclusion interaction between self-assembled pyrenyl-nanofibrils and γ -cyclodextrins (γ -CDs). The amphiphilic pyrenyl derivatives display the self-assembled nanofibrils in aqueous media, providing the hydrophobic π -extended conjugated system at the inner part and hydrophilic functionality at the periphery. Their monomeric components are captured by γ -CDs, which decompose nanofibrils to form a dimer of Py-CO2: γ -CD complexes. Finally, it is shown that nanofibrils are re-formed as the γ -CD is decomposed by α -amylase. These structural changes drive highly selective and sensitive detection of α -amylase at very low concentrations by ratiometric fluorescence color changes.

Poster Presentation : **ORGN.P-612**

Organic Chemistry

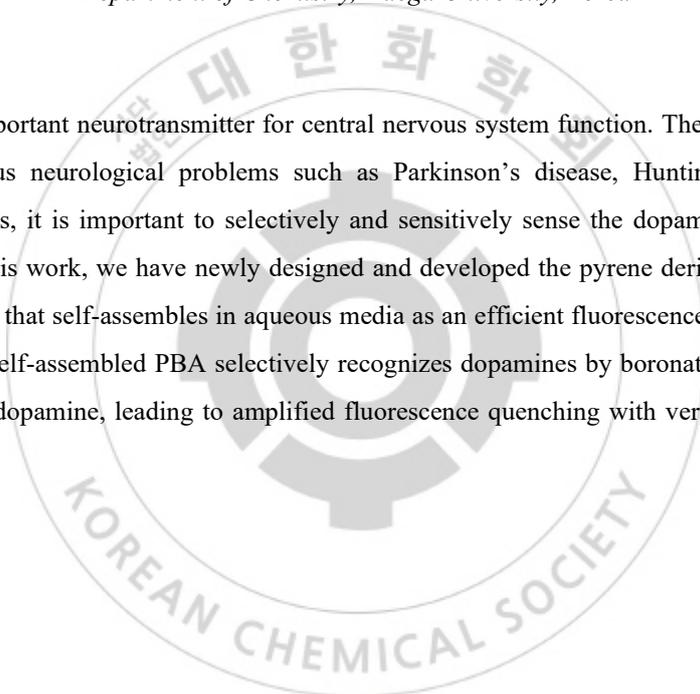
Zoom 15 FRI 15:00~16:00

A Micelle-based fluorescent probe for efficient detection of dopamine

HyeBin Song, Seoung Ho Lee*

Department of Chemistry, Daegu University, Korea

Dopamine is an important neurotransmitter for central nervous system function. The abnormal dopamine level causes various neurological problems such as Parkinson's disease, Huntington's disease, and Schizophrenia. Thus, it is important to selectively and sensitively sense the dopamine concentration in human serum. In this work, we have newly designed and developed the pyrene derivative with a phenyl boronic acid (PBA) that self-assembles in aqueous media as an efficient fluorescence sensor for detection of dopamine. The self-assembled PBA selectively recognizes dopamines by boronate-catechol formation between PBA and dopamine, leading to amplified fluorescence quenching with very high Stern-Volmer constants.



Poster Presentation : **ORGN.P-613**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

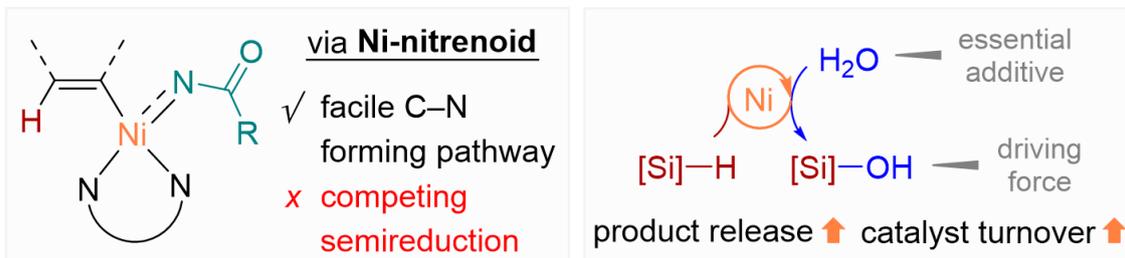
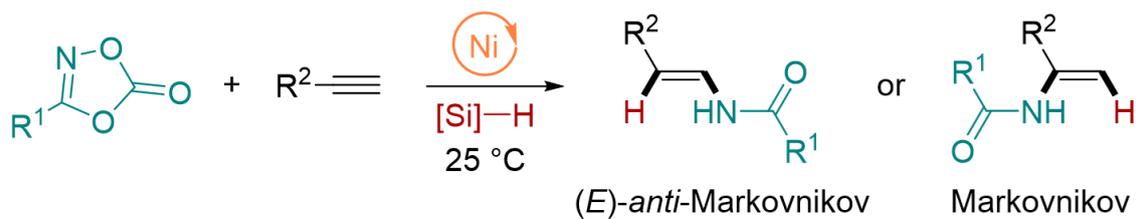
Merging NiH Catalysis and Inner-Sphere Metal-Nitrenoid Transfer for Hydroamidation of Alkynes

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 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 H₂O 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. The virtue of this strategy is demonstrated by sequential reduction of an underexplored class of secondary enamides that are challenging to obtain otherwise.



Poster Presentation : **ORGN.P-614**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

Catalytic Enantioselective Acyloin Rearrangement of Aldehydes Using Chiral Oxazaborolidinium Ion

Soo Min Cho, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Acyloin rearrangement, involving 1,2-aryl or alkyl migration to the carbonyl group, is a useful synthetic method for synthesis of α -hydroxy ketone (acyloin), which is a versatile building block for many natural products and pharmaceuticals.^[1] To overcome inherent reversibility of this reaction in equilibrium, the enantioselective acyloin rearrangements of aldehyde moieties have been developed.^[2] The reaction of aldehyde moieties undergoes a unidirectional equilibrium toward ketone products, because of thermodynamic advantage compared to aldehydes.^[3] Using this strategy, there is only one examples of catalytic asymmetric acyloin rearrangements of acyclic aldehyde.^[4] Because this methodology provided acyloins in low yield (11-54%) with 74-88% ee, however, the development of a new catalytic reaction is highly desired. In this research, we developed a catalytic enantioselective acyloin rearrangement of acyclic aldehydes with broad applicability. Using chiral oxazaborolidinium ion (COBI) catalysts as Lewis acid, highly optically active acyloins were obtained in excellent yields (up to 95%) with excellent enantioselectivities (up to 98%).**References**[1] S.-H. Wang, B.-S. Li, and Y.-Q. Tu. Chem. Commun. (2014) 50, 2393.[2] (a) H. Wu, Q. Wang, and J. Zhu. Angew. Chem. Int. Ed. (2017) 56, 5858. (b) X. Zhang, R. J. Staples, A. L. Rheingold, and W. D. Wulff. J. Am. Chem. Soc. (2014) 136, 13971. (c) T. Ooi, K. Ohmatsu, and K. Maruoka. J. Am. Chem. Soc. (2007) 129, 2410.[3] L. A. Paquette and J. E. Hofferberth Organic Reactions. Vol. 62, Wiley, Hoboken, (2003) pp. 477-525.[4] L. Dai, X. Li, Z. Zeng, S. Dong, Y. Zhou, X. Liu, and X. Feng. Org. Lett. (2020) 22, 5041.

Poster Presentation : **ORGN.P-615**

Organic Chemistry

Zoom 15 FRI 15:00~16:00

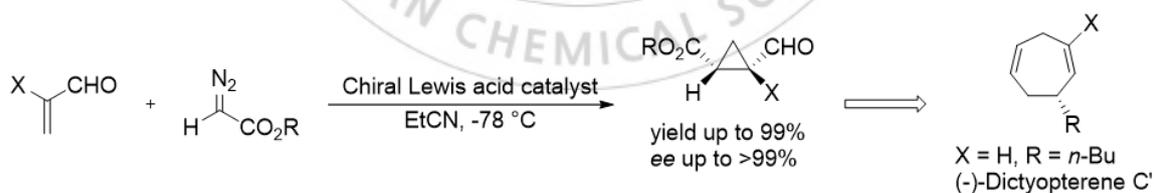
Enantioselective Synthesis of 1,4-Cycloheptadiens from Chiral Boron-based Lewis Acid Catalyzed Enantioselective Cyclopropanation

Kyung Yee Park, Do Hyun Ryu^{1,*}

Chemistry, Sungkyunkwan University, Korea

¹*Department of Chemistry, Sungkyunkwan University, Korea*

Cyclopropane skeleton is a key structure found in various bioactive molecules and natural products. Among various cyclopropane compounds, chiral cyclopropanes which contain two carbonyl groups have been studied and synthesized through various reactions such as transition-metal-catalyzed reactions and ylide-based cyclopropanation. Compared to synthetic methods of *trans*-dicarbonyl cyclopropanes, synthetic method of *cis*-dicarbonyl cyclopropanes has rarely been reported. Herein, we describe enantioselective cyclopropanation from α , β -unsaturated aldehydes and alkyl diazoacetates using chiral boron-based Lewis acid catalyst. Using this synthetic method, we synthesized (-)-Dictyoptereine C' and its derivatives containing 1,4-cycloheptadienes from *cis*-dicarbonyl cyclopropanes.



Poster Presentation : **ORGN.P-616**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Modular Tuning of Electrophilic Reactivity of Iridium Nitrenoids for the Intermolecular Selective α -Amidation of β -Keto Esters

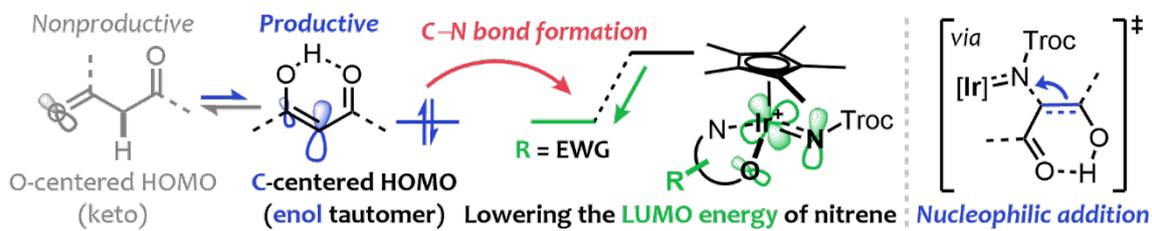
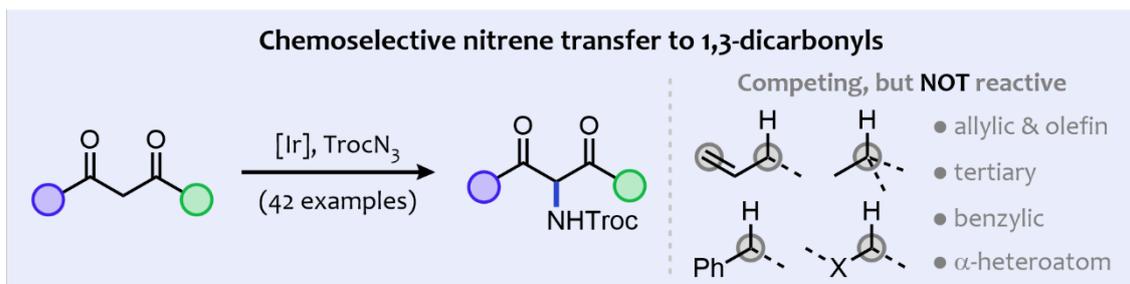
Minhan Lee, Hoimin Jung, Dongwook Kim¹, Jung-Woo Park^{2,*}, Sukbok Chang^{*}

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

¹*Center for Catalytic Hydrocarbon Functionalization, Institute for Basic Science, Korea*

²*Department of Chemistry, Institute for Basic Science, Korea*

The α -amination of carbonyl compounds has attracted significant attention as a route for creating building blocks for applications in natural products and pharmaceuticals. Because the α -carbonyl carbon and amine reactants are electronically mismatched, this reaction requires a polarity reversal of components to enable C–N bond formation at the α -position. To accomplish this, researchers have relied on pregenerated 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. Toward that end, we reported a highly selective α -amination of 1,3- dicarbonyl compounds using iridium carbonylnitrenes as electrophilic animating species. Using TrocN₃ as the amino source, the electrophilic nature of the iridium-nitrenoid intermediate was modulated by electronically tuning the κ^2 -N,O ligands, leading to C–N bond formation by nucleophilic addition of enol π -bonds. This mechanistic approach, supported by both experimental and computational evidence, could be used to enhance reaction efficiency as well as chemoselectivity in a nitrene transfer process, providing a platform for the future development of animation reactions for a variety of applications in synthetic and medicinal chemistry.



Poster Presentation : **ORGN.P-617**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Enantioselective epoxidation with diazo ester catalyzed by chiral Lewis acid catalyst.

Dong Guk Nam, Do Hyun Ryu*

Department of Chemistry, Sungkyunkwan University, Korea

Optically active epoxides and its derivatives are versatile building blocks and powerful intermediates in modern organic synthesis because of their synthetic utilities that they can be ring-opened with a wide range of nucleophiles with complete stereoselectivity and regioselectivity. Especially, synthesis of chiral epoxy ketones were highly desirable because the highly functionalized enantiomeric enriched trisubstituted epoxy ketone that have the potential to be highly valuable synthetic intermediates for various synthesis. A highly diastereo- and enantioselective method for the epoxidation of glyoxals with diazoester has been developed for the synthesis of a variety chiral α,β -Epoxy Ketone. In the presence of a catalyst, the reaction proceeded with good yields (up to 99%) with excellent enantioselectivities (up to >99% ee) and with single diastereomer.

Poster Presentation : **ORGN.P-618**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

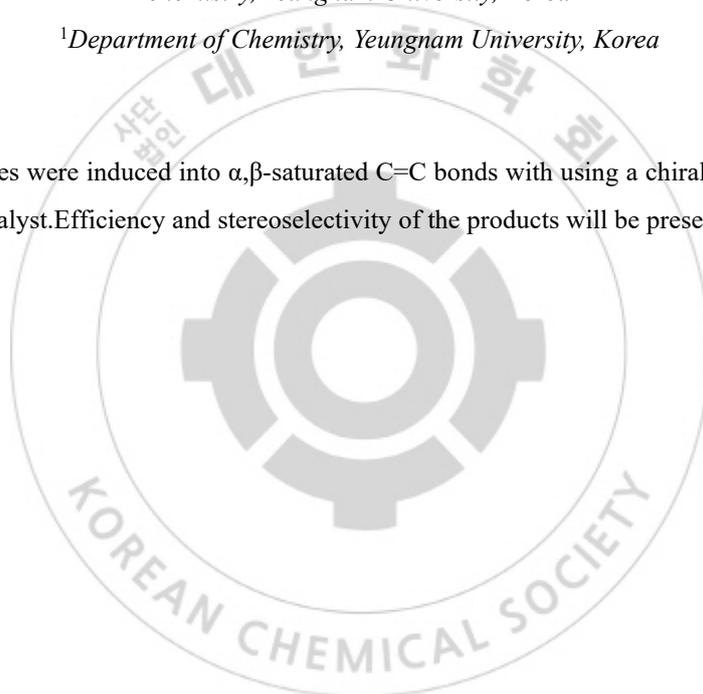
Synthesis of Asymmetric Amino Acid Derivatives: Michael Addition

Hyunsoo Oh, Keehyung Nahm^{1,*}

chemistry, Yeungnam University, Korea

¹*Department of Chemistry, Yeungnam University, Korea*

Several Nucleophiles were induced into α,β -saturated C=C bonds with using a chiral cinchona catalyst as a phase transfer catalyst. Efficiency and stereoselectivity of the products will be presented.



Poster Presentation : **ORGN.P-619**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Aggregation-induced emission scaffold Kaleidolizine for mitochondria-targeted photodynamic therapy

Sang-Kee Choi, Eunha Kim*

Department of Molecular Science and Technology, Ajou University, Korea

Development of photodynamic therapy (PDT) have been provided an efficient noninvasive treatment modality for diverse cancer treatment. Excitation of a photosensitizers followed by intersystem crossing(ISC) from the lowest singlet excited state(S1) to the lowest triplet excited state(T1) generates the reactive oxygen species, which damage the organelles and trigger the cell death. Conventional photosensitizers such as phorphyrin and cyanine structures are suffering from intrinsic aggregation caused quenching(ACQ) that reduces singlet oxygen (1O_2) generation in aqueous media, resulting in low efficiency of PDT performance. For newly developed class of photosensitizers, aggregation-induced emission(AIE) fluorophore can elaborate a new solution for highly selective and limited to specific legion. By changing the substituent having different electron density, it can control the energy gap between S1 and T1 intersystem crossing affecting to 1O_2 generation and more efficient PDT[1]. From previous studies, indolizine based fluorogenic scaffold[2] is able to overcome the ACQ problem as a AIE fluorophore scaffold. In this work, we modify 3 sites of the indolizine core to give diverse electron density to control the Δ EST Gap which can affect the PDT effect. Keywords : Photodynamic Therapy, Indolizine, AIE, Fluorophore

Poster Presentation : **ORGN.P-620**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Ring-Opening Functionalizations of Unstrained Cyclic Amines Enabled by Difluorocarbene Transfer

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Institute for Basic Science, Korea

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

Chemical synthesis based on the skeletal variation has been prolifically utilized as an attractive approach for modification of molecular properties. Given the ubiquity of unstrained cyclic amines, the ability to directly alter such motifs would grant an efficient platform to access unique chemical space. Here, we report a highly efficient and practical strategy that enables the selective ring-opening functionalization of unstrained cyclic amines. The use of difluorocarbene leads to a wide variety of multifaceted acyclic architectures, which can be further diversified to a range of distinctive homologative cyclic scaffolds. The virtue of this deconstructive strategy is demonstrated by successful modification of several natural products and pharmaceutical analogues.

Poster Presentation : **ORGN.P-621**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

High-Valent Rh Catalysis for Mild C–H Acyloxylation via Electro-Oxidation

Seongho Jin, Jinwoo Kim¹, Sukbok Chang*

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

¹Center for Catalytic Hydrocarbon Functionalizations, Institute for Basic Science, Korea

Despite of high importance of C–O bond construction, its formation via oxidative coupling has been hampered by high energy barrier for the reductive elimination process which requires harsh reaction conditions or excess amount of the reaction partner. Disclosed here is that oxidation of cyclometalated Cp*Rh(III) carboxylate intermediate dramatically decreases the reductive elimination barrier to facilitate C–O bond formation. The electro-oxidation readily affords the high-valent Rh(V) dicarboxylate intermediate leading to the development of mild C–H oxygenation method using stoichiometric amounts of carboxylate reaction partner.

Poster Presentation : **ORGN.P-622**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Hydrophobic Superbase Catalysis to Access Functional Alkylsulfur(VI) Fluorides “On-Water”

Jin Hyun Park, Han Yong Bae*

Department of Chemistry, Sungkyunkwan University, Korea

The sulfur(VI) fluoride exchange (SuFEx) reaction, which was revived by Sharpless and co-workers, is identified as a remarkably powerful next generation “click chemistry” that enables absolute reliable connectivity.¹ Among efficient SuFExable hubs, ethenesulfonyl fluoride (ESF) and β -aryl-substituted ESFs are regarded as obviously useful new-type functionalized olefins. Those utilities had drawn considerable attention from chemical biology and molecular pharmacology. Despite sustained attention, however, successful functionalization of β -aryl-substituted ESFs via Michael addition reaction is still elusive because of their intrinsic low electrophilicities and untamed side transformations. We recently discovered “on-water” catalysis enables surprising rate acceleration due to the hydrophobic hydration effect.² In a confined hydrophobic shell, high spatial proximity between substrates and catalyst tremendously reinforces desired transformations.³ Herein, by taking advantage of the powerful water-induced reactivity amplification, we disclose an efficient catalytic protocol to access thioester incorporated SuFExable Hubs. Unprecedented “on-water” organo-superbase catalyst triggers Michael addition reaction of dithiomalonate to β -substituted ESFs to provide desired γ -geminal dithioester bearing sulfonyl fluorides (up to 99% yield).⁴ Previously applied catalytic systems failed to achieve the desired transformation due to unselective decay of sulfonyl fluoride functional group.

Poster Presentation : **ORGN.P-623**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

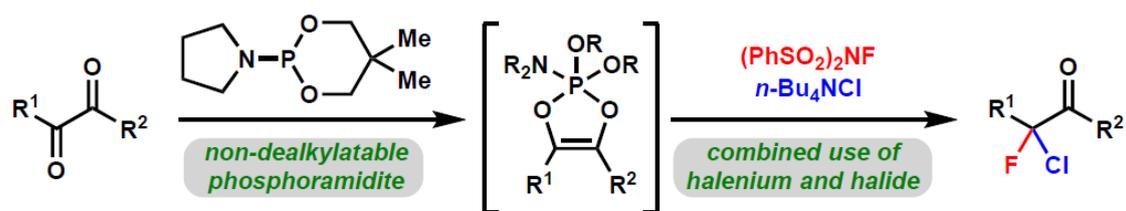
Phosphorus(III)-Mediated, Tandem Deoxygenative Geminal Chlorofluorination of 1,2-Diketones

Ha Eun Kim, Won-jin Chung*

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

Halogenation of organic compounds is one of the most important transformations in synthetic chemistry. In particular, tetrasubstituted carbons containing two different halogens are useful synthetic precursors.¹ However, most of the synthetic methods for geminal interhalogenation of the α -position of a carbonyl group have been limited to sequential electrophilic halogenations. This traditional method requires a two-step process, and it is difficult to avoid the unwanted overhalogenated side product, which is hard to separate. Here, we describe a conceptually distinct method for geminal chlorofluorination that avoids those problems via tandem electrophilic and nucleophilic halogenation on the same carbon.² In this work, dioxaphospholene, known as the Kukhtin–Ramirez adduct, was employed as a carbene surrogate. Through the design of a non-dealkylatable phosphoramidite, the formation of geminal chlorofluoride was enabled from bench-stable 1,2-diketones with *N*-fluorobenzenesulfonimide (NFSI) and tetra-*n*-butylammonium chloride. The reaction provided geminal chlorofluorides in up to 88% yield for aryl-aryl 1,2-diketones and up to 71% yield for aryl-alkyl 1,2-diketones. In addition, a selective functionalization of the chlorine substituent was demonstrated.

References 1.(a) Cresswell, A. J.; Eey, S. T.-C.; Denmark, S. E. *Angew. Chem., Int. Ed.* **2015**, *54*, 15642–15682; (b) Chung, W.-j.; Vanderwal, C. D. *Angew. Chem., Int. Ed.* **2016**, *55*, 4396–4434.
2. Choi, G.; Kim, H. E.; Hwang, S.; Jang, H., Chung, W.-j. *Org. Lett.* **2020**, *22*, 4190–4195.



- dioxaphospholene as carbene surrogate
- tandem, one-step gem-chlorofluorination
- no halogen scrambling



Poster Presentation : **ORGN.P-624**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Effect of Terminal Groups on the Helical Structure of Unnatural β -Peptides

Junyeong Jeong, Soo Hyuk Choi^{1,*}

Department of Chemistry, Yonsei University, 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-625**

Organic Chemistry

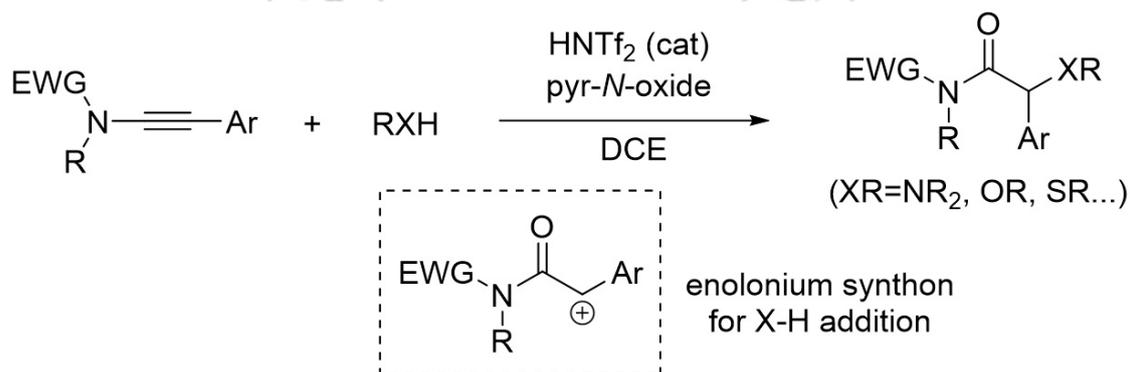
Zoom 15 FRI 16:00~17:00

Brønsted Acid Catalyzed Oxidative Coupling Reaction of Ynamides with Heteroatom-nucleophiles

Tae-Woong Um, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Synthesis of α -heteroatom substituted carbonyl compounds is important because an array of pharmaceuticals and bioactive compounds contain this moiety. Oxidative functionalization of ynamides can lead to unpoled enolonium synthons and a number of protocols have been reported for the addition of C-nucleophiles. However, addition of heteroatom-nucleophiles have seen only limited success, so far. In this presentation, we disclose addition of hetero-atom nucleophiles on the ynamide-derived enoloniums, encompassing alcohols, hydrazides, anilines, and aryl/alkyl thiols. Key to the success of this hetero-functionalization is a chemoselective oxidation that are compatible with many of the nucleophiles.



Poster Presentation : **ORGN.P-626**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Carbofluorination of Allenamide via an α -Fluorinated Iminium Intermediate

Hae Eun Lee, Jin Kyoong Park*

Department of Chemistry, Pusan National University, Korea

Fluorine atoms are found in about 30% of agrochemicals such as herbicides and fungicides. Besides, fluorinated compounds are key chemicals in pharmaceutical synthesis, materials, and polymer science because of their properties such as permeability, metabolic stability, and lipophilicity. To install fluorine atoms, fluorofunctionalization has been considered one of the most straightforward strategies. Therefore, many synthetic chemists have developed elegant methods for carbofluorination under metal-catalyzed or metal-free reaction conditions. Recently, we discovered the general carbofluorination reactions of allenamides using selectfluor under milder conditions. The fluorinated iminium was characterized and utilized for one-pot carbofluorination by adding TMS-protected carbon moieties. We have successfully explored almost 50 examples of substrate scopes and were able to synthesize diverse organic building blocks such as skipped enynes, 1,4-dienes, 1,5-dienes, and functionalized enamines.

Poster Presentation : **ORGN.P-627**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

A process for the direct water-free synthesis of common ionic liquids: microwave-assisted continuous flow technology

Lei Cao, Jin Kyoong Park^{1,*}

Chemistry, Pusan National University, Korea

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

One-step efficient alkyl halide-free synthesis of ionic liquids was performed under the assistance of microwave and continuous flow technology in the presence of alkyl orthoformate with acid. A wide range of imidazole, pyridine, and tertiary amine derivatives rapidly reacted with trimethyl, triethyl, tripropyl and tributyl orthoformate using various Brønsted acid or ammonium salt to control anion parts, such as BF₄⁻, PF₆⁻, OTs⁻, N(Tf)₂⁻, NO₃⁻, OTf⁻, Cl⁻, Br⁻, and I⁻, under microwave batch condition, forming corresponding ionic liquids in excellent yields mostly within 10 min. For comparison, the reaction took more than 17 h with conventional thermal transfer heating. Notably, DMF used as solvent contributed to the formation of ionic liquids especially when aliphatic tertiary amine derivatives were used as reactants. Besides small molecules, poly(vinylimidazole) and poly(vinylpyridine) successfully converted to corresponding polyionic liquids indicating the application in the modification of polymer surface. Large scale (gram scale) synthesis was easily approached in a microwave flow system. Also, the excess of orthoformate could be collected and reused by distillation resulting low E factor of 0.8. For easier setup, the whole process could be carried out in a household microwave. Low waste production and efficient productivity support a further extensive application.

Poster Presentation : **ORGN.P-628**

Organic Chemistry

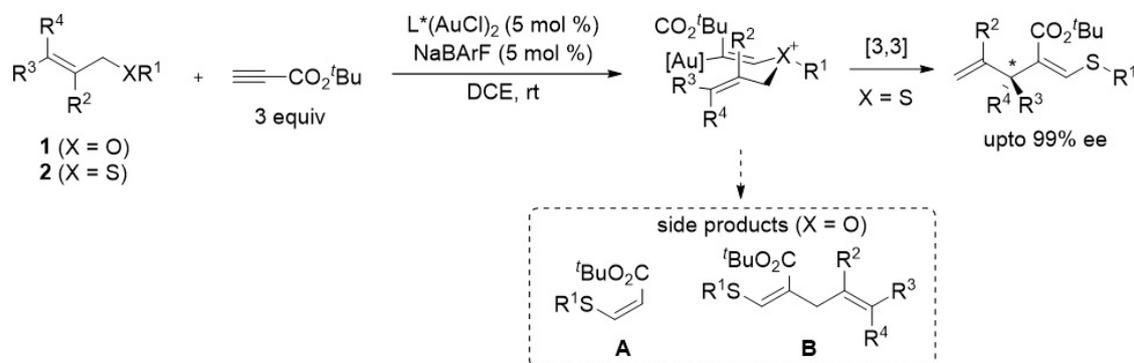
Zoom 15 FRI 16:00~17:00

Gold(I)-Catalyzed Enantioselective Thioallylation of Propiolates via Charge-Induced Thio-Claisen rearrangement

Jiwon Jang, Seunghoon Shin*

Department of Chemistry, Hanyang University, Korea

Enantioselective intermolecular gold-catalysis is challenging, because the linear coordination geometry of Au(I) complexes imposes the approach of pronucleophiles from the opposite side of the gold. Prompted by our recent success in promoting intermolecular enantioselective coupling of propiolates and alkenes, we embarked on the enantioselective alkoxylation and thioallylation of propiolates, via [3,3]-sigmatropic rearrangement. The substrate scope of enantioselective Claisen rearrangement has been limited to a few systems and we introduced herein use of -onium intermediates for the enantioselective Claisen rearrangement for the first time. Remarkably, by replacing allyl ethers with allyl thioethers, problems such as dissociation of allyl unit (A) and competing [1,3]-rearrangement (B) could be minimized. Thus, the current Au(I)-catalyzed thioallylation allows for remarkable scope of allyl group, including highly enantioselective synthesis of all C-quaternary centers and exceptional functional group compatibility with many Lewis bases and π -groups.



Poster Presentation : **ORGN.P-629**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

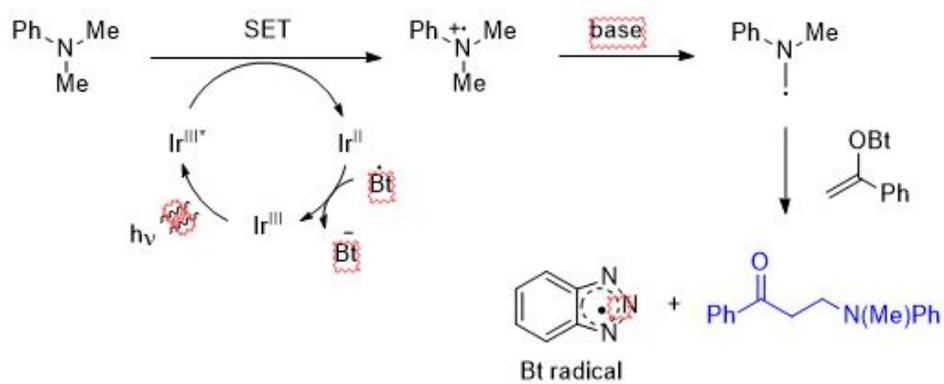
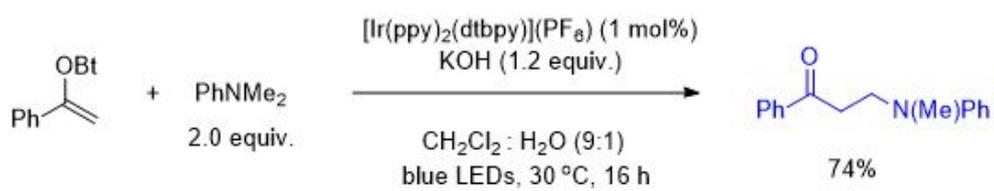
Photoredox Reactivity of *N*-Enoxybenzotriazole Enabled Radical Mannich Reaction via sp^3 C-H Bond Functionalization of Tertiary Amines

Huong Quynh Nguyen, Seunghoon Shin^{1,*}

Chemistry, Hanyang University, Korea

¹*Department of Chemistry, Hanyang University, Korea*

Over the past few decades, harnessing of one-electron reactivity from visible light catalysis has emerged as an appealing tool to access radical intermediates, enabling C-C and C-X bond formations. In continuation of our interest in the N-O bond-mediated oxidative transformations, we introduce herein enoxybenzotriazoles as substrates for the photo-catalyzed radical Mannich type reaction of tertiary amines. We envisioned that functionalization of C(sp^3)-H bond amine by single electron transfer would generate N-centered radical cation which is deprotonated to produce an α -amino radical. The newly formed radical then reacted with a molecule of N-enoxybenzotriazole substrate furnishing β -amino ketone product and benzotriazole radical (Bt radical). Bt radical oxidized Ir^{II} back to the photoreactive Ir^{III} specie and complete the catalyst cycle.



Poster Presentation : **ORGN.P-630**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Structural Influence of Terminal Functional Groups on TEGBased Leveler in Microvia Filling

Jung Ah Kim, Young gyu Kim*

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

To develop high density interconnection (HDI) in electronics, Copper electrodeposition has been used for microvia filling in printed circuit board (PCB) and integrated circuits (IC). Since it is important to achieve defect-free and seam-less filling, several organic additives are used in Cu deposition. Leveler is one of the additives used in electroplating process to promote homogenous surface deposition through its convection-dependent adsorption behavior. In previous research, the structure of levelers showed relation with the inhibition effect of levelers. Thus, studying structure-property relationship in leveler will help to understand mechanisms and future design of levelers. In this research, we devised the general structure of leveler: ammonium groups with halide counter ions, ethylene glycol unit, and hydroxyl groups besides the carbon chains. These functional groups have several effective features in Cu^{2+} reduction in past studies. Upon this structure, we synthesized triethylene glycol (TEG)-based levelers with different terminal groups and compared their influences on inhibition effect. The structure-property relationship of these levelers was investigated through electrochemical analyses as linear sweep voltammetry (LSV).

Poster Presentation : **ORGN.P-631**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Oxidative Ring Contraction of 1,4-Dimethoxyphthalazines via *N*-Chlorination

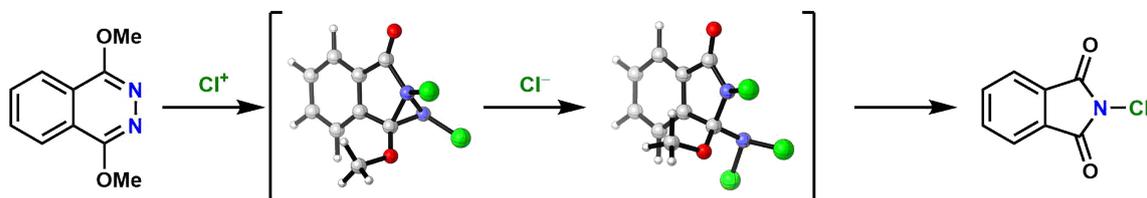
Iju Jeong, Won-jin Chung*

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

A rarely observed *N*-chlorination induced, oxidative ring contraction of 1,2-diazines was studied. The reaction of 1,4-dimethoxyphthalazine derivatives with trichloroisocyanuric acid (TCICA) afforded the ring contraction product, *N*-chlorophthalimides. The addition of an exogenous chloride was found to effectively accelerate the ring contraction. From the isolated monochlorinated intermediate, a bicyclization/ring-opening mechanism was proposed for this unprecedented ring contraction and supported by DFT calculation. Furthermore, the additional examination of several other electrophilic reagents only revealed the unique promoting ability of TCICA.

References

1. J. K. Im, B. Yang, I. Jeong, J.-H. Choi, W.-j. Chung, *Tetrahedron Lett.* **2020**, *61*, 152048.
2. J. K. Im, I. Jeong, B. Yang, H. Moon, J.-H. Choi, W.-j. Chung, *Synthesis* **2021**, *53*, DOI: 10.1055/s-0040-1706639.



- ◆ Chlorenium-promoted ring contraction
- ◆ Bicyclization/ring-opening mechanism
- ◆ Elimination of a nitrogen fragment

Poster Presentation : **ORGN.P-632**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

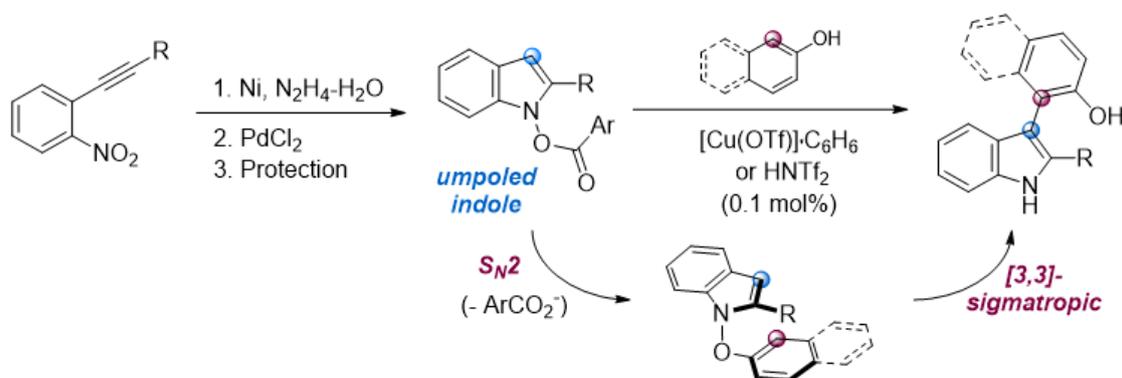
***Ortho*-Selective C-H Arylation of Phenols with Electrophilic Indoles**

Nguyen Nguyen, Seunghoon Shin^{1,*}

Hanyang University, Vietnam

¹*Department of Chemistry, Hanyang University, Korea*

Direct functionalization of inert C-H bonds is an attractive strategy and therefore have drawn intense interest. To implement such a strategy for regioselective functionalization of phenols, we introduced herein *N*-benzoylindoles as electrophilic, unpoled indole derivatives. However, direct oxidation of indoles is difficult, due to the strong aromaticity, and their synthesis have typically resorted to tedious reduction and oxidation sequences. Therefore, in this presentation, an efficient and general synthesis of *N*-acyloxyindoles based on electrophilic cyclization of (*o*-alkynyl)phenylhydroxylamines was introduced. With the unpoled indole derivatives in hand, two catalytic systems for *ortho*-selective coupling with phenols were developed, namely HNTf₂ and [Cu(OTf)]·C₆H₆. While HNTf₂ catalyst provided a metal-free protocol, [Cu(OTf)]₂·C₆H₆ proved to be extremely powerful, catalyzing the reaction at ambient temperature with as low as 0.01 mol% of the catalyst. The unusual *ortho*-regioselectivity was rationalized by a sequence comprising N-O bond forming by S_N2 substitution with phenols, followed by [3,3]-sigmatropic rearrangement.



Poster Presentation : **ORGN.P-633**

Organic Chemistry

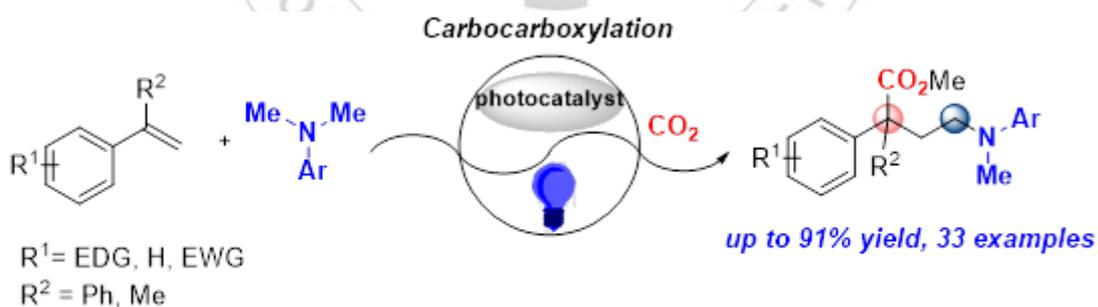
Zoom 15 FRI 16:00~17:00

Transition Metal-Free Carbocarboxylation of Styrenes with CO₂ via Visible-Light Photoredox Catalysis

Hyungwoo Hahm, Sukwon Hong*

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

γ -aminobutyric acid (GABA) is the main inhibitory neurotransmitter in the mammalian central nervous system (CNS).[1] For this reason, the synthesis of various γ -aminobutyric acid derivatives has been considered important in the pharmaceutical field.[2] Over the past several years, photoredox catalysis for C-C bond formation with CO₂ has been extensively studied.[3] However, photoredox-catalyzed difunctionalization of alkenes with CO₂ is rare.[4] Herein, we will discuss visible-light-mediated carbocarboxylation of alkenes with CO₂ and tertiary amines using organophotocatalyst for γ -aminobutyric esters synthesis. This reaction is a broad range of substrate scope.



- γ -aminobutyric ester
- Broad substrate scope
- High regioselectivity
- Mild condition

Poster Presentation : **ORGN.P-634**

Organic Chemistry

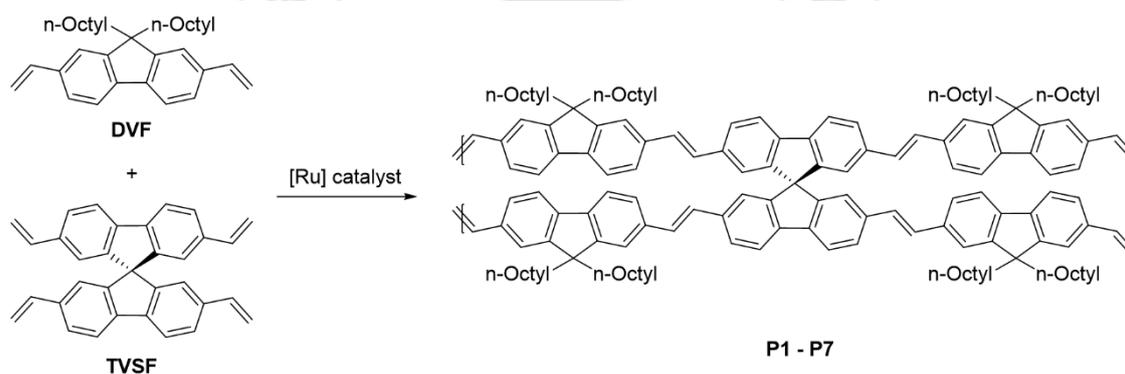
Zoom 15 FRI 16:00~17:00

Synthesis of Conjugated Copolymers by Acyclic Diene Metathesis Polymerization for Light-emitting Diodes Applications

Seongwook Park, Sukwon Hong*

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

Grubbs-type, Hoveyda-type, cyclic alkyl amino carbene (CAAC)-based ruthenium olefin metathesis catalysts were used for the acyclic diene metathesis (ADMET) polymerization of 2,7-divinyl-9,9-di-n-octylfluorene (DVF). Additionally, various ratios DVF and 2,2',7,7'-tetravinyl-9,9'-spirobifluorene (TVSF) were used to ADMET polymerization to obtain copolymer P1-P7. The polymers were analyzed with gel permeation chromatography, UV-vis spectroscopy, and photoluminescence spectroscopy. Polymer light-emitting diode (PLED) devices were fabricated with polymers.



Poster Presentation : **ORGN.P-635**

Organic Chemistry

Zoom 15 FRI 16:00~17:00

Relative conformation and stability of the D,L-alternating octapeptides depending on β -residue types

Hyerim Yoon, Soo Hyuk Choi*

Department of Chemistry, Yonsei University, Korea

Unlike most of the proteins and peptides found in nature only consist of L-amino acids, some microorganisms have peptides containing D-amino acids. In particular, D/L- peptides are natural peptides consisting of alternating sequences of D-amino acids and L-amino acids. This peptide has high physiological activity and is known to form several β -helix conformations, different from conventional protein secondary structures. DL-Oligomer structures consisting only of D/L-Val have been studied in an interesting way. The introduction of β -amino acids is known to form a more stable and fixed helix structure than that of α -amino acids present in the natural world. We design a DL-peptide that introduces cyclohexane-based β -amino acid to D residues to mimic D/L-Val oligomer. Octamer-length candidate peptides were designed by replacing them with β -amino acids to form similar β -helix conformation at shorter lengths with lower molecular weights than natural D/L-peptides. We synthesized D-/L- peptide forming a specific β -helix structure, such as double helical structure or channel structure. Also, we confirmed the structural tendency through IR, CD and single X-ray crystallography. Next, we characterized of D-/L- peptide helices with cyclic or acyclic β -residue. We synthesized D/L-peptides containing acyclic β^2 -residue and studied that has a specific folding conformation in all solvent. It was studied that various β -amino acids could be introduced and we can control β -helix structure depending on stimulation and environments.

Poster Presentation : **MEDI.P-636**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Real-time imaging of virus infection using a graphene oxide-based nanosensor to repurpose antiviral agents

Hojeong Shin, Dal-Hee Min*

Department of Chemistry, Seoul National University, Korea

Dengue virus (DENV) is one of the most prevalent arthropod-borne viruses that belongs to the genus Flavivirus. DENV is a serious human pathogen that threatens global public health. Although the severe progression of DENV infection can cause life-threatening complications, there are no approved therapeutics to treat DENV infection yet. Thus, there is an unmet need for the discovery of effective medications against DENV. To address this need for anti-DENV therapy, we developed a graphene oxide-based fluorescent nanobiosensor (Graphene Oxide-based Viral RNA Analysis system, GOViRA) that can be used for antiviral drug screening. The GOViRA system is composed of GO and fluorescent PNA probe which is complementary to the target viral RNA. They can selectively recognize the target genome and facilitate the quantitative analysis of the intracellular viral genome. We successfully applied the GOViRA platform to high-throughput antiviral screening and identified a potent inhibitor against DENV infection that has anti-DENV activity both in vitro and in vivo.

Poster Presentation : **MEDI.P-637**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Solid-Phase Synthesis of thiazolo[4,5-*d*] pyrimidine derivatives via Intramolecular Cyclization

Su jin Lim, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

Fused heterocycles are one of the most attractive compounds in drug discovery field due to their various biological activities. Over the years, fused pyrimidine systems including thiazolo[4,5-*d*]pyrimidine have shown various biological activities such as antitumor, antiviral, anticancer, etc. In this study, we were interested in the synthesis of thiazolo[4,5-*d*]pyrimidine derivatives via solid phase approach using traceless linker on Merrifield resin. First, the cyclization of cyanocarbonimidodithioate terminated resin with bromoacetonitrile would provide 4-amino-thiazole-5-carbonitrile intermediate. Next, imination of the intermediate with *N,N*-dimethylformamide dimethyl acetal with following treatment with various amines gives our desired thiazolo[4,5-*d*]pyrimidine core skeletons. Diversification is proceeded with a number of electrophiles like acyl chlorides, alkyl halides. Interestingly, the acylation step shows the effect of protection of amine positioned in thiazolo[4,5-*d*] pyrimidine preventing oxidation of the secondary amine. The phenomenon occurs only for compounds with aromatic amines. After the cleavage from the resin, protection group was also removed resulting in increased yields of thiazolo[4,5-*d*]pyrimidine derivatives. Resins reacted with alkyl halides, acyl chlorides underwent oxidation with mCPBA and following cleavage from the resin via amines provides diverse library of thiazolo[4,5-*d*]pyrimidine derivatives. Finally, we confirmed the oral bioavailability of the library by the calculation of the physicochemical properties.

Poster Presentation : **MEDI.P-638**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Progress in discovery of a selective Hsp90 degrader

Hak Joong Kim^{*}, Sehee Cha

Department of Chemistry, Korea University, Korea

Heat shock protein 90 (Hsp90) is an essential molecular chaperon in eukaryotes engaged in folding, stabilization, and degradation of over 400 client proteins. In addition, when a cell faces a stress such as heat shock, expression of Hsp90 is increased to minimize cellular damage. Many of the client proteins are oncogenes; 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 as well as off-target toxicity. Proteolysis targeting chimera (PROTAC) is a strategy to selectively degrade protein of interest (POI) by inducing ubiquitination on POI. It depends on the use of a heterobifunctional molecule composed of covalently linked ligands for POI and E3 ligase, which increases the proximity between POI and the E3 ligase. Due to the unique mode of action, PROTAC strategy is considered as a promising alternative to traditional inhibitor-based therapeutics. In this poster, we present our progress in synthesis and evaluation of PROTAC compounds targeting Hsp90. Our discussion will be focused on whether a PROTAC approach can provide an alternative solution to the problems of currently available Hsp90 inhibitors encountered during their development as anti-cancer agents.

Poster Presentation : **MEDI.P-639**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Identification of novel inhibitors of Monoamine oxidase-B (MAO-B)

Euijung Kim, Wooyoung Hur^{1,*}

Department of Chemistry, Korea University, Korea

¹*Chemical Kinomics Research Center, Korea Institute of Science and Technology, Korea*

Monoamine oxidase are a family of enzymes that perform oxidation of monoamines. MAOs play vital role in the inactivation of neurotransmitters. MAO-A mainly metabolizes the tyramine and MAO-B catalyzes the oxidative deamination of dopamine. Motor symptoms of parkinson's disease are caused by extensive loss of dopaminergic neurons resulting in nigrostriatal dopamine deficiency. Accordingly, MAO-B inhibitors dopamine degradation in nigrostriatal pathway and could be developed as drugs to modulate Parkinson's disease. Here, we performed an in silico screening using machine learning method against about 100,000 small molecule library. Forty-two compounds were purchased and surprisingly 5 of them showed IC₅₀s of less than 100 nM against human MAO-B. All of the 5 hits exhibited >100 selectivity over human MAO-A. We picked up 2 hits and synthesized analogues to identify selective, potent MAO-B inhibitors. We wish to demonstrate the powerfulness of AI-driven virtual screening as a tool to streamline the hit identification process and disclose structure-activity relationship of our hit compounds.

Poster Presentation : **MEDI.P-640**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Development of practical synthetic process for iodinated radiocontrast agents

Kyungmin Kim, KangJoo Lee, Sun-Joon Min^{1,*}

Applied Chemistry, Hanyang University, Korea

¹*Dept of Chemical & Molecular Eng/Applied Chemistry, Hanyang University, Korea*

As X-ray technology is widely used as a medical imaging tool for detection of pathology, radiocontrast agents have been developed as key substances for improving the visibility of imaging. Among them, 5-amino 2,4,6-triiodoisophthalic acid derivatives was first announced in 1974 as one of the most traditional contrast agents, and it has been used as a diagnostic agent for CT (computed tomography) protocols since 1981. Most recently, it has been studied that it could be applicable to a combined CT and MRI (magnetic resonance imaging) protocol. This material is stable in animal and human experiments with high tolerability and low toxicity. In particular, it is useful for angiography via cardiovascular system, and it can be easily removed due to rapid excretion from the kidney. A typical industrial process for 5-amino 2,4,6-triiodoisophthalic acid derivatives is involved in three-step reaction sequences including coupling with optically active 2-acetoxypyrrolidinone, amide formation with serinol, and ester hydrolysis, starting from readily available 5-amino-2,4,6-triiodoisophthaloyl dichloride. In this process, optical purity might be reduced due to epimerization under basic condition. Additionally, the final product should be isolated after filtration with a large excess of resin, which can increase the production cost. In this study, we present a practical and efficient synthetic process of this radiocontrast agent by way of serinol derivatives. This new method will be applied to manufacturing process in a pharmaceutical company in due course.

Poster Presentation : **MEDI.P-641**

Medicinal Chemistry

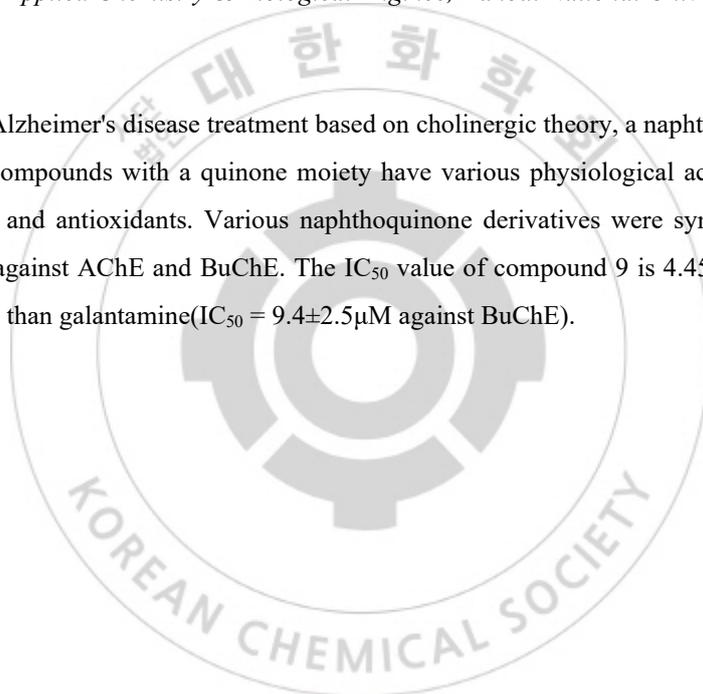
Zoom 16 FRI 15:00~16:00

Naphthoquinone derivatives for Butyrylcholinesterase Inhibitor

Junhyeong Lee^{*}, Ji hyun Hwang^{*}, Jiyeon Lee, Jeong Ho Park^{*}

Division of Applied Chemistry & Biological Enginee, Hanbat National University, Korea

To develop a new Alzheimer's disease treatment based on cholinergic theory, a naphthoquinone derivative was synthesized. Compounds with a quinone moiety have various physiological activities such as anti-cancer, antibiotics, and antioxidants. Various naphthoquinone derivatives were synthesized to measure inhibitory activity against AChE and BuChE. The IC_{50} value of compound 9 is $4.45 \pm 0.84 \mu M$, it is more effective IC_{50} value than galantamine($IC_{50} = 9.4 \pm 2.5 \mu M$ against BuChE).



Poster Presentation : **MEDI.P-642**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

1,3,4-Oxadiazole-2(3H)-thione analogs as PIM Kinase Inhibitors

Seungik Jeong, Hyeonseong Choo, Jinho Lee*, Victor Sukbong Hong*

Department of Chemistry, Keimyung University, Korea

Proviral integration site for moloney murine leukemia virus (PIM) kinases are highly expressed in hematological, pancreatic and colon cancers. PIM kinases are a family of serine/threonine kinases composed of three different isoforms, PIM1, PIM2 and PIM3. Each of the PIM kinases phosphorylates downstream substrates that contributes to tumor growth and survival. The small molecular pan-Pim kinase inhibitors are currently the focus of intensive drug development efforts. In the present study, 1,3,4-oxadiazole-2(3H)-thione and indole conjugates were designed and the structural features that affect their potency were investigated. Structure–activity relationship studies yielded potent inhibitors of all three PIM kinases in the single-digit to low double-digit nanomolar IC₅₀ range. Kinase profiling of a representative compound showed high selectivity among 15 other kinases.

Poster Presentation : **MEDI.P-643**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

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*

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 synthesis starts from the cyclization of the 1-(2-hydroxy-5-nitrophenyl)ethanone with 1-Boc-4-piperidon in the presence of pyrrolidine. After reduction of the keto group, mesylation with methane sulfonyl chloride resulted in methanesulfonates, and a double bond could be formed by DBU induced elimination of mesyl group. Following deprotection of tert-butyloxycarbonyl protecting group and conversion of the nitro group to primary amine were performed. Thus, the functionalization of the core skeleton can be performed on both amino groups. Diversification was performed using various sulfonyl chlorides and alkyl halides via standard protocols. After diversification, a diverse library of *N*-alkyl-1'-(substituted sulfonyl)spiro[chromene-2,4'-piperidin]-6-amine was obtained. The library is expected to be checked for its anti-inflammatory inhibitory activity.

Poster Presentation : **MEDI.P-644**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Solid-Phase Synthesis of Thiazolo[4,5-*b*]azepine-5,10-dione Derivatives via Intramolecular Cyclization

Dana Kim, Young Dae Gong*

Department of Chemistry, Dongguk University, Korea

The fused heterocycles are one of the most attractive compounds in drug discovery field due to their various biological activities. For instance, fused azepinediones have shown various biological activities such as antitumor, DGAT1 inhibition, etc. In this study, we were interested in the synthesis of thiazolo[4,5-*b*]azepine-5,10-dione derivatives via solid phase approach. First, the reaction of thiourea terminated resin and ethyl 2-(2-bromoacetyl)benzoate would provide valuable ethyl 2-(4-aminothiazole-5-carbonyl)benzoate intermediate. Next, the cyclized ethyl 2-(4-aminothiazole-5-carbonyl)benzoate resin could undergo intramolecular cyclization with further functionalization using various electrophiles like alkyl halides, acid chlorides to give a range number of N-substitued aminothiazoloazepine compounds. After cleavage off the resin, we expect to obtain diverse library of thiazolo[4,5-*b*]azepine-5,10-dione derivatives.

Poster Presentation : **MEDI.P-645**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Design, Synthesis, Biological Evaluation of TAZ inhibitors for anticancer drug

Moon gyu Baek, Eul Kgun Yum*, Kwan-Young Jung^{1,*}

Department of Chemistry, Chungnam National University, Korea

¹Drug Discovery Platform Research Center, Korea Research Institute of Chemical Technology, Korea

The hippo pathway has been shown to be a major signaling pathway that regulates various biological functions, and the function of the hippo pathway regulates organ size by blocking cell proliferation and promoting cell apoptosis. However, due to a malfunction in the regulation of the hippo pathway, the oncogene protein TAZ, a downstream factor of the hippo pathway, interacts with the TEA domain transcription factor to inhibit cancer cell apoptosis and promote cancer cell proliferation. In addition, excessive activation of TAZ causes tissue abnormal proliferation and human cancer, and pharmacological interference with the activity of TAZ-TEA domain transcription factor could be a new strategy for anticancer therapy. Currently, there are a few small molecules developed for the protein TAZ, and related researches are ongoing. Among TAZ inhibitors, the most potent inhibitor is niflumic acid. The carboxylic acid of niflumic acid forms a hydrogen bond with the Cysteine 380 and the Valine 347 is in contact with the pyridine moiety, showing that it is an important functional group. Therefore, our study introduced the pyridine scaffold of niflumic acid, designed and synthesized 50 different derivatives. Structure activity relationship (SAR) studies confirmed that the inhibitory activity of the para-substituent was increased rather than the meta-substituent of benzene moiety. The results showed that among the synthesized derivatives, compound 49 showed 100% inhibitory activity against the interaction of the TAZ-TEA domain transcription factor and proved that it is a more potent inhibitor than niflumic acid.

Poster Presentation : **MEDI.P-646**

Medicinal Chemistry

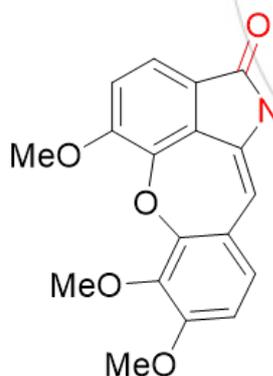
Zoom 16 FRI 15:00~16:00

Synthesis and Evaluation of New Benzoxepinoindol-1-ones as a Brd4 Inhibitor

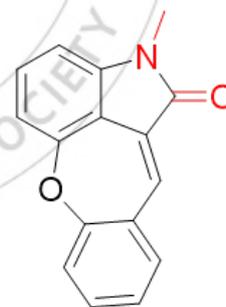
Goni Jung, Eunyoung Yoon*, Jung-Nyoung Heo*

Center for Medicinal Chemistry, Korea Research Institute of Chemical Technology, Korea

Novel benzo[6,7]oxepino[4,3,2-cd]indolone derivatives have been designed and synthesized based on Aristoyagonine structure, which is known as an inhibitor of Brd4 (Bromodomain-containing protein 4). The core 7-membered oxepin ring was constructed using aldol condensation and S_NAr reaction between 4-hydroxy-1-methylindolin-2-ones and 2-halobenzaldehydes. Benzoxepinoindol-1-ones will be examined their biological activities as an anticancer agent.



Aristoyagonine
Brd4 IC_{50} = 0.8 μ M



Benzo[6,7]oxepino[4,3,2-cd]indolone

Poster Presentation : **MEDI.P-647**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Development of QSAR methods for predicting immunotoxicity targeting T and B-lymphoblast

Hyeon Ki Kim, Dong Ryeol Shin, Sung Kwang Lee*

Department of Chemistry, Hannam University, Korea

Immunotoxic compound reduces resistance to infectious agents or autoimmune diseases by suppressing or enhancing the immune response. QSAR studies to predict the toxicity of compounds are steadily progressing, but QSAR research on immunotoxicity of compounds is a field that is rarely studied due to the complexity of its toxicity. In this study, we developed QSAR models that can quickly predict immunotoxicity from various atomic fragments based on the growth inhibition data from the NCI-60 database (data for CCRF-CEM, MOLT-4 cell lines targeting T-lymphocytes and data for RPMI-8226 cell line targeting B-lymphocytes). Various atomic fragments that can classify the toxicophores were generated by Morgan molecular fingerprint, and the redundant fragments and the fragments not related to immunotoxicity were excluded through the Chi square value. We implemented a QSAR (Quantitative structure activity relationship) model using naive bayes, XGBoost, and lightGBM as model algorithms from the filtered data set. The best model made using CCRF-CEM, MOLT-4, and RPMI-8226 data, respectively, had an AUC value of 0.8 or higher and an F-measure of 0.6 or higher for both the validation set and the test set. The Bayesian score in the Bayesian model and the weight of features in the tree-based models (XGBoost and lightGBM) could indicate the major substructure that inhibit the growth of each lymphoblast. Acknowledgment : This research was supported by a grant (20183 대체기 524-3) from the Ministry of Food and Drug Safety in 2021.

Poster Presentation : **MEDI.P-648**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Activatable fluorescent probes for the development of cleavable linker releasing a drug

Dong-Jo Chang

Department of Pharmacy, Suncheon National University, Korea

Ligand targeted-drug delivery has been developed for the enhancement of selective localization of small molecule drugs or imaging agents into tumor tissues. In ligand-targeted drugs, a targeting ligand 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 specifically binding to malignant antigens have been considered as a vehicle to selectively deliver a cargo including cytotoxic or imaging agents to target cells as shown in antibody-drug conjugates (ADCs). In this study, we provide a model study for the development of cleavable linker using the activatable fluorescent probes releasing a fluorophore by the response to a 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-aminobenzyl spacer. The comparative analysis for the stability and effect of linkages and spacer on the fluorophore release was provided by the quantitative kinetic study on enzymatic assay and cell-based assay in HepG2 cells, and the stability of the leucine linker conjugated via various linkages and spacer was evaluated ex vivo by estimating fluorescence emitted in plasma, which can provide a simple protocol for the analysis of plasma stability of linker.

Poster Presentation : **MEDI.P-649**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

The biological activities of supercritical fluid extract (SPE) of the green propolis

Bong Ho Lee^{*}, Byong Wook Choi¹

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

¹Department of Chemical & Biological Engineering, Hanbat National University, Korea

Propolis is known to have diverse biological activities such as antioxidative, anti-inflammatory, enzyme(s) inhibitory activities and thus it is used in various commercial products. Extracts from propolis, used in food, pharmaceutical and cosmetic industries, present quality and composition related to the extraction method applied. We prepared supercritical fluid extracts (SPE) from Brazilian propolis and screened them for their biological activities such as antioxidative, antiinflammatory, and enzyme inhibitory activities Brazilian green propolis supercritical extraction at different temperature (35 - 60 °C) and pressure (150 - 400 bar). The yields were less than 10 % and changed with extraction conditions. The water-EtOH extract showed strong DPPH radical scavenging activity as expected and the supercritical fluid extract showed lower radical scavenging activity. Both The water-EtOH propolis extract and SPE showed weak NO synthase inhibitory activities at 5 µg/ml and two SPE showed weak IL-6 synthesis inhibitory activity. The water-EtOH extract showed weak collagenase inhibitory activity less than 10 % at 5 µg/ml and SPE showed moderate collagenase inhibitory activity at the same concentration. These results support the other literature data, the supercritical fluid extract of propolis contains less polar components such as terpenoids. The novel results for green propolis found in this study show that it is possible to obtain extracts with antioxidative, anti-inflammatory, and enzyme inhibitory potential using a clean technology under the defined conditions.

Poster Presentation : **MEDI.P-650**

Medicinal Chemistry

Zoom 16 FRI 15:00~16:00

Analysis of lysine and arginine blockers for site-selective trypsin digestion

Kunal More, Dong-Jo Chang*

Department of Pharmacy, Suncheon National University, Korea

Site-selective chemical modification of amino acids is important in the field of chemical biology, shotgun proteomics, and the production of peptide drugs. Although different chemical modifying agents for site-selective modification of amino acids are widely reported, the extent and site selectivity of the modification of specific amino acids is yet to be examined. Thus, in this regard, a method to determine the extent and site selectivity would be very useful. In this report, as a novel method to determine the extent of site-selective chemical modification of amino acid fluorogenic peptide substrate (MeRho-Lys/Arg-Gly-Leu) and the proteolytic enzyme trypsin-based model study was performed. In the context of proteolysis by trypsin, the fluorogenic peptide substrate produces fluorescence owing to site-selective cleavage at either arginine or lysine, whereas modification of proteolytic site arginine or lysine decreases the fluorescence. The extent of amino acid modification is expressed in terms of half-maximal inhibitory concentrations (IC₅₀) and site selectivity is evaluated from ratios of IC₅₀ values (IC₅₀arginine/IC₅₀lysine and IC₅₀lysine/IC₅₀arginine). This novel method was found very useful for accurate determinations of the extent and site selectivity of chemical modification.

Poster Presentation : **MEDI.P-651**

Medicinal Chemistry

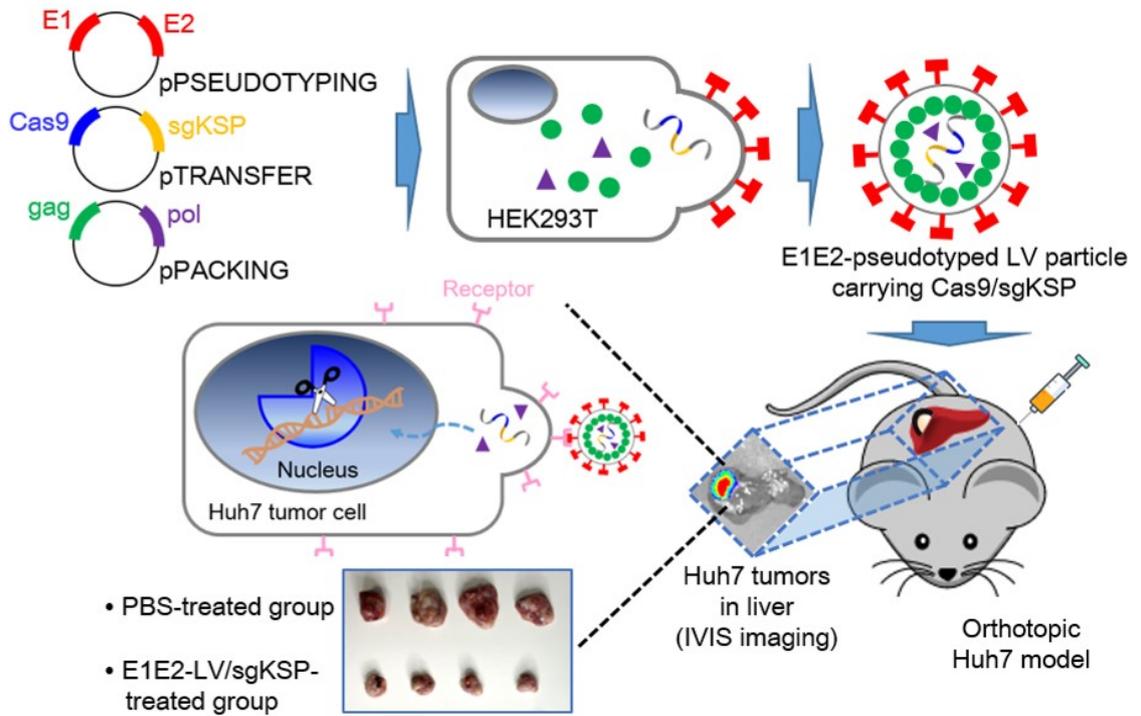
Zoom 16 FRI 16:00~17:00

Systemic Delivery of CRISPR/Cas9 to Hepatic Tumors Using Altered Tropism of Lentiviral Vector in Cancer Therapy

Hyung Jun Ahn

Theragnosis, Korea Institute of Science and Technology, Korea

Therapeutic application of CRISPR/Cas9 nucleases remains a challenge due to the lack of efficient in vivo delivery carriers. Here, we examine the ability of lentiviral vectors pseudotyped with hepatitis C virus (HCV)/E1E2 envelope glycoproteins to systemically deliver CRISPR/Cas9 to hepatic tumors in vivo. We demonstrated that systemic administration of E1E2-pseudotyped lentiviral vectors can selectively deliver Cas9 and sgRNA specific for kinesin spindle protein (KSP) to Huh7 tumors in the orthotopic Huh7 mice due to the specific interactions between E1E2 and their cellular receptors. This specific delivery leads to effective KSP gene disruption, potently inhibiting tumor growth. Furthermore, we demonstrated that E1E2-pseudotyping is more suitable for systemic delivery of CRISPR/Cas9 in cancer therapy than vesicular stomatitis virus-pseudotyping, the most widely used pseudotyping, because of stability in human serum, little transduction to DCs, low innate immune response, and cell-specific targeting ability. This study suggests that E1E2-pseudotyped lentivirus carrying CRISPR/Cas9 can substantially benefit the treatment of Huh7 tumors.



Poster Presentation : **MEDI.P-652**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

KCP10043F induces cell death in non-small cell lung cancer (NSCLC) through apoptosis induction via the reduced phosphorylated STAT3.

Minji Kang, Dohyeong Ko, Gwang Hyun Moon, JunSeong Ahn, Jae Yeol Lee*

Department of Chemistry, Kyung Hee University, Korea

We previously reported that 4-(4-fluorobenzylcarbamoylmethyl)-3-(4-cyclohexylphenyl)-2-[3-(N,N-dimethylureido)-N'-methylpropylamino]-3,4-dihydroquinazoline (KCP10043F) can induce G1-phase arrest and synergistic cell death in combination with etoposide in lung cancer cells. Here, we investigated the underlying mechanism by which KCP10043F induces cell death in non-small cell lung cancer (NSCLC). Propidium iodide (PI) and annexin V staining revealed that KCP10043F-induced cytotoxicity was caused by apoptosis. KCP10043F induced a series of intracellular events: (1) downregulation of Bcl-2 and Bcl-xL and upregulation of Bax and cleaved Bid; (2) loss of mitochondrial membrane potential; (3) increase of cytochrome c release; (4) cleavage of procaspase-8, procaspase-9, procaspase-3, and poly (ADP-ribose) polymerase (PARP). In addition, KCP10043F exhibited potent inhibitory effects on constitutive or interleukin-6 (IL-6)-induced signal transducer and activator of transcription (STAT3) phosphorylation and STAT3-regulated genes including survivin, Mcl-1, and cyclin D1. Furthermore, STAT3 overexpression attenuated KCP10043F-induced apoptosis and the cleavage of caspase-9, caspase-3, and PARP. Docking analysis disclosed that KCP10043F could bind to a pocket in the SH2 domain of STAT3 and prevent STAT3 phosphorylation. The oral administration of KCP10043F decreased tumor growth in an A549 xenograft mouse model, as associated with the reduced phosphorylated STAT3, survivin, Mcl-1, and Bcl-2 expression and increased TUNEL staining and PARP cleavage in tumor tissues. Collectively, our data suggest that KCP10043F suppresses NSCLC cell growth through apoptosis induction via STAT3 inactivation.

Poster Presentation : **MEDI.P-653**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

***N*-Amido-phenylsulfonamide Derivatives as Potent and Selective Microsomal Prostaglandin E₂ Synthase-1 (mPGES-1) Inhibitors**

Geuntae Kim, Yunchan Nam, Seyoung Yang, Jiwon Woo, Jae Yeol Lee*

Department of Chemistry, Kyung Hee University, Korea

Our previous research showed that *N*-carboxy-phenylsulfonyl hydrazide (scaffold A) could reduce LPS-stimulated PGE₂ levels in RAW 264.7 macrophage cells by an inhibition of mPGES-1 enzyme. However, a number of scaffold A derivatives showed drawbacks such as the formation of regioisomers and poor liver metabolic stability. To overcome these synthetic and metabolic problems, we decided to replace *N*-carboxy-phenylsulfonyl hydrazide (scaffold A) with *N*-carboxy-phenylsulfonamide (scaffold B) or *N*-amido-phenylsulfonamide (scaffold C) as a bioisosteric replacement. Among them, **MPO-0186** (scaffold C) inhibited the production of PGE₂ (IC₅₀: 0.24 μM) in A549 cells via inhibition of mPGES-1 (IC₅₀: 0.49 μM in a cell-free assay) and was found to be approximately 8 to 9-fold more potent than a reference inhibitor, **MK-886**. A molecular docking study theoretically suggests that **MPO-0186** could inhibit PGE₂ production by blocking the PGH₂ binding site of mPGES-1 enzyme. Furthermore, **MPO-0186** demonstrated good liver metabolic stability and no significant inhibition observed in clinically relevant CYP isoforms. This result provides a potential starting point for the development of selective and potent mPGES-1 inhibitor with a novel scaffold.

Poster Presentation : **MEDI.P-654**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

PROTAC-induced cIAP2/XIAP protein degradation ; Design, synthesis, and in vivo efficacy studies

Dayoung Kim, Hyunjin Kim^{1,*}

Department of Pharmacy, Sungkyunkwan University, Korea

¹*Bio & Drug Discovery Division, Korea Research Institute of Chemical Technology, Korea*

In recent years, a novel and effective technology so-called “proteolysis targeting chimeras” (PROTACs) has been actively studied in the field of drug development. PROTAC strategy employs the targeted protein degradation machinery of the cancer cell ; the ubiquitin-proteasome pathway. Degradation of the protein as using PROTACs pathway is targeted for deletion by the attachment of a polyubiquitin chain which leads to their recognition and subsequent degradation by the 26S proteasome. The PROTAC molecule include a ligand binding an E3 ubiquitin ligase which is connected by a linker to another ligand binding the target protein. The association between a protein and an E3 ligase, as induced by a PROTAC molecule, will result in the transfer of ubiquitin and degradation of the targeted protein. As part of our efforts to design and study novel PROTAC-based small molecule inhibitors, we were interested in IAP as a targeted protein due to its distinct role in cells. Here we report the synthesis and activities of thalidomide-based IAP degraders.

Poster Presentation : **MEDI.P-655**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

Total synthesis of phlebiarubrone and its derivatives for the development of natural product pharmaceuticals

Cheol Hee Yoon^{*}, Jiyoool Kim¹, Pilju Choi², Taejung Kim³, Jungyeob Ham³

chemistry, Korea Institute of Science and Technology, 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*

Recently, natural products obtained from the nature exhibit a lot of biological activities and it sometimes become to the lead compound for drugs. For example, natural products and its derivatives such as taxol, vincristine, morphine and codeine are already used as anticancer drugs and anodynia, and so on. Especially, these natural products are suitable in terms of safety for human, therefore, drug development from natural products has received much attentions in the world. Focusing on new drug development, we have been continuing to synthesize pharmacophores of natural products including biological activities and further modifying them to functionalized derivatives. Also, to further enhance effective methods to find natural product derivatives, our research has applied to the concept of Naturomimetic Approach developed by our group. Biologically active pharmacophore of natural product is synthesized and efficient research to find further moiety is conducted through Pd-catalyzed carbon-carbon coupling reactions. In the poster presentation, we will introduce our recent research results in Naturomimetic Approach from mushroom-derived p-terphenyl natural product as a therapeutic agent for inflammatory diseases.

Poster Presentation : **MEDI.P-656**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

An improved approach of the synthesis of natural 1-arylnaphthalene lactones via Hauser–Kraus naphthol formation strategy

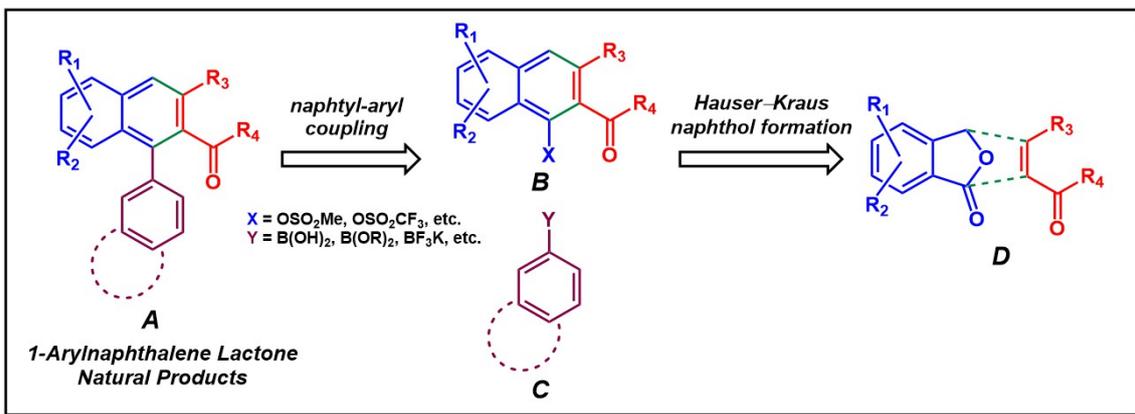
Jiyool Kim^{*}, Cheol Hee Yoon¹, Young-Tae Park², Taejung Kim², Jungyeob Ham²

biological chemistry, university of science and technology, Korea

¹*chemistry, Korea Institute of Science and Technology, Korea*

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1-Arylnaphthalene lactones are a subgroup of the lignan class of molecules characterized by a phenylpropanoid dimer motif. Many of these natural 1-arylnaphthalene lactone lignans have attracted considerable attention with the discovery of intriguing antiviral, anticancer, antiplatelet, piscicidal and antibacterial properties. New natural products within this class of compounds continue to be reported, and ongoing studies have led to a better understanding of their biosynthetic origins with the hopes of finding a viable biotechnological production methodology. However, previous methods are limited in obtaining a variety of 1-arylnaphthalene lactone natural products and in the preparation of these derivatives by replace aryl moiety with heterocycle or carbonyl-containing aryl group for pharmaceutical drug discovery. If this type coupling reaction were to proceed between sulfonate B (derived from precursor D) and boron aryl compound C, various 1-arylnaphthalene lactone lignans A would be synthesized in a few steps with the involvement of Hauser–Kraus naphthol formation from phthalides. In this poster, detailed experimental results about our original approach of the synthesis and biological evaluation of natural 1-arylnaphthalene lactone lignans will be disclosed.



Poster Presentation : **MEDI.P-657**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

Protopanaxadiol type ginsenosides Rk1 and Rg5 inhibit lung cancer migration and invasion.

Haneul Ju^{*}, Pilju Choi¹, Young-Tae Park¹, Jungyeob Ham¹, Chung-Min Park²

Natural Products Research, Gangneung-Wonju National University, Korea

¹*Natural Products Research, Korea Institute of Science and Technology, Korea*

²*Chemical Advanced Materials, Gangneung-Wonju National University, Korea*

Lung cancer has a high incidence worldwide, and most lung cancer-associated deaths are attributable to cancer metastasis. The prerequisites for starting metastasis is the migration and invasion of cancer, which is very important in cancer metastasis because it's the earliest process. Transcription factors that regulate epithelial-mesenchymal transition (EMT) have been identified in many malignant cancers. Recent research shows EMT is linked to the formation of stem cells from differentiated cancer cells. Panax ginseng Meyer, the root of *P. ginseng* has been used as functional food and herbal medicine for thousands of years worldwide, especially in Korea and China, owing to its medicinal properties. The biologically active components of ginseng are called ginsenosides. There are several methods for enhancing the bioactive properties of ginseng. In an earlier study, we had described the conversion of ginsenosides by microwave-thermal processing to improve the bioactive properties of ginseng. Ginseng extract using microwave contains a lot of ginsenoside Rg3, Rk1 and Rg5. Although several studies have reported anticancer effects of Rg3, the effects of Rk1 and Rg5 on cancer progression are relatively unknown. In this study, we investigated the anticancer effects of Rk1 and Rg5 on TGF- β 1 accelerated EMT in A549 cells.

Poster Presentation : **MEDI.P-658**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

Synthesis of lithocholic acid derivatives and its biological activity

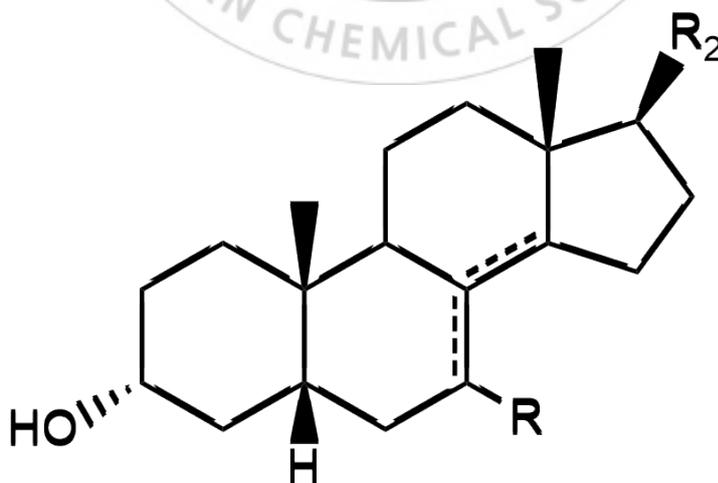
Soobin Park, Dowon Yoon¹, Jung Woog Kim, Hakwon Kim^{2,*}

Kyung Hee University, Korea

¹*Applied Chemistry, Kyung Hee University, Korea*

²*Department of Applied Chemistry, Kyung Hee University, Korea*

The bile acids, cholic acids (CA), are steroid acids found predominantly in the bile of mammals and other vertebrates. Diverse bile acids are formed from cholesterol in the liver of mammals. They have a physiological function to help in the digestion of lipids and lipophilic vitamins reabsorption. Among bile acid derivatives, lithocholic acid (LCA) has recently shown drug formulation-stabilizing and anti-inflammatory effects. In this study, we were particularly interested in the anti-inflammatory activity of LCA, so we synthesized several LCA derivatives and investigated their anti-inflammatory activity. In addition, to determine the difference in anti-inflammatory activity according to the structure of the LCA derivatives, we compared with the activity of LCA.



general structures of Lithocholic acid derivatives

Poster Presentation : **MEDI.P-659**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

Design and Synthesis of Novel Template, Truncated 1'-Homologated 4'-Thioadenosine Derivatives as Pure Dual PPAR γ / δ Modulators

Zijing Liu, Gyudong Kim*

College of Pharmacy, Chonnam National University, Korea

Following our report that A3 adenosine receptor (AR) antagonist exhibited a polypharmacological profile as a dual modulator of peroxisome proliferator-activated receptor (PPAR) γ / δ , we discovered a new template, 1'-homologated 4'-thioadenosine analogues, as dual PPAR γ / δ modulators without AR binding. Removal of binding affinity to A3AR was achieved by 1'-homologation, and PPAR γ / δ dual modulation was derived from the structural similarity between the target nucleosides and PPAR modulator drug, rosiglitazone. All the final nucleosides were devoid of AR-binding affinity and exhibited high binding affinities to PPAR γ / δ but lacked PPAR α binding. 2-Cl derivatives exhibited dual receptor-binding affinity to PPAR γ / δ , which was absent for the corresponding 2-H derivatives. 2-Propynyl substitution prevented PPAR δ -binding affinity but preserved PPAR γ affinity, indicating that the C2 position defines a pharmacophore for selective PPAR γ ligand designs. PPAR γ / δ dual modulators functioning as both PPAR γ partial agonists and PPAR δ antagonists promoted adiponectin production, suggesting their therapeutic potential against hypoadiponectinemia-associated cancer and metabolic diseases.

Poster Presentation : **MEDI.P-660**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

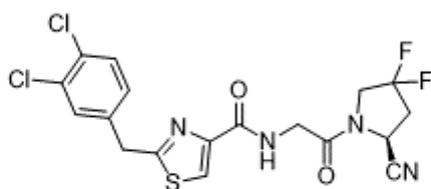
Identification of BR102910 as a selective fibroblast activation protein (FAP) inhibitor

Hui jin Jung, In Su Kim^{1,*}, Youjung Byun¹

Department of Medicinal chemistry , Boryung Pharmaceutical, Korea

¹*College of Pharmacy / Department of Pharmacy, Sungkyunkwan University, Korea*

Fibroblast activation protein (FAP) is a member of the serine protease DPP family of enzymes, consisting of DPP 4, FAP, DPP 2, DPP 8, DPP 9, and PREP, and shares 52% amino acid identity with DPP 4. FAP has dual activities with both a post-proline dipeptidase and an endopeptidase. FAP is expressed at the sites of tissue remodeling and also activates the hepatocytes. Based on these findings, several FAP inhibitors have been reported, showing increased levels of intact FGF21 with improved insulin resistance. In the present study, we explored in detail the structure–activity relationship around several heteroaryl scaffolds and extensively optimized compounds that displayed highly satisfactory inhibitory potency and high selectivity against the related DPP4 and prolyl oligopeptidase (PREP). Among optimized compounds, BR102910 showed low nanomolar potency, high selectivity and excellent in vitro ADMET profiles such as microsomal stability, plasma stability, CYP inhibition and hERG. Additionally pharmacokinetic evaluation in mice of BR102910 demonstrated exceptional PK profiles and favorable FAP inhibition efficacy. Based on these excellent in vitro/in vivo profiles, further development studies are planned to evaluate the potential of BR102910 as a highly potent and selective FAP inhibitor.



<BR102910>↵

(S)-N-(2-(2-cyano-4,4-difluoropyrrolidin-1-yl)-2-oxoethyl)↵
-2-(3,4-dichlorobenzyl)thiazole-4-carboxamide↵



Poster Presentation : **MEDI.P-661**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

Design and Synthesis of Novel Template, Truncated 1'-Homologated Oxacyclic Adenosine Derivatives as Pure Dual PPAR γ / δ Modulators

Juri Jeong, Gyudong Kim*

College of Pharmacy, Chonnam National University, Korea

Following our report that A₃ adenosine receptor (AR) antagonist exhibited a polypharmacological profile as a dual modulator of peroxisome proliferator-activated receptor (PPAR) γ / δ , we discovered a new template, 1'-homologated oxacyclic adenosine analogues 4a–4h, as dual PPAR γ / δ modulators without AR binding. Removal of binding affinity to A₃AR was achieved by 1'-homologation, and PPAR γ / δ dual modulation was derived from the structural similarity between the target nucleosides and PPAR modulator drug, rosiglitazone. All the final nucleosides were devoid of AR-binding affinity and exhibited high binding affinities to PPAR γ / δ but lacked PPAR α binding. 2-Cl derivatives exhibited dual receptor-binding affinity to PPAR γ / δ , which was absent for the corresponding 2-H derivatives. PPAR γ / δ dual modulators functioning as both PPAR γ partial agonists and PPAR δ antagonists promoted adiponectin production, suggesting their therapeutic potential against hypoadiponectinemia-associated cancer and metabolic diseases.

Poster Presentation : **MEDI.P-662**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

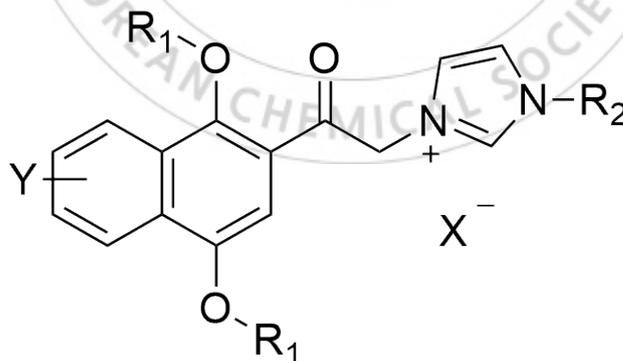
Synthesis of 1,4-dialkoxynaphthalen-2-acyl imidazolium salts and its antifungal activity

Haena Lee, Hyejin Moon, Hakwon Kim^{1,*}

Kyung Hee University, Korea

¹*Department of Applied Chemistry, Kyung Hee University, Korea*

Even though *Candida* sp. is a common residue of human skin, it is also an opportunistic pathogenic fungus that can cause candidiasis. The emergence of resistant *Candida* strains and the toxicity of antifungal agents have encouraged the development of new classes of potent antifungal agents. Therefore, in this study, we designed and synthesized novel naphthalen-2-acyl imidazolium salts (NAIMSs), especially 1,4-dialkoxy-NAIMS from 1,4-dihydroxynaphthalene and tested their antifungal activity by micro-dilution anti-fungal susceptibility testing (MIC assay).



Novel naphthalen-2-acyl imidazolium salts (NAIMSs)

Poster Presentation : **MEDI.P-663**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

Synthesis and evaluation of anti-microbial adjuvant agents that enhance the potency of aminoglycosides

So eun Park, Hak Joong Kim^{1,*}

Chemistry, Korea University, Korea

¹*Department of Chemistry, Korea University, Korea*

Antibacterial agents have been used since the 1940s and saved the lives of many people. However, these drugs were so abused, and thereby resistant bacteria emerged rapidly. As one way to circumvent this phenomenon, anti-bacterial adjuvant agents have been investigated. These agents are used to repotentiate the existing antibiotics no longer effective against drug-resistant bacteria. Specifically, our laboratory has been focused on finding an adjuvant molecule effective for *Acinetobacter baumannii*. This is a gram-negative bacterium belonging to opportunistic pathogens. The issue of infection by *A. baumannii* is serious problem because of significant antibiotic resistance, which significantly limits the range of therapeutic options. Herein, a newly discovered antimicrobial adjuvant agent “CC-236096” as well as related derivatives that can reduce resistance of *A. baumannii* to aminoglycoside antibiotics were studied. *A. baumannii* is not susceptible to kanamycin up to 512 µg/mL, but upon treatment of 0.312 µg/mL CC-236096, for instance, the minimal inhibitory concentration (MIC) of kanamycin has dropped to 16 µg/mL. Even when used alone, some analogues could display decent potency of MIC 0.625 µg/mL, suggesting that it can be a new antibiotic candidate as well. This poster presentation shows our preliminary structure-activity study as well as future plans for structural optimization.

Poster Presentation : **MEDI.P-664**

Medicinal Chemistry

Zoom 16 FRI 16:00~17:00

Discovery of Novel Tau Aggregation Inhibitors for the Treatment of Alzheimer's Disease

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¹*Convergence Research Center for Diagnosis, Treatment and Care System of Dementia, Korea*

Alzheimer's disease is a chronic neurodegenerative disease. In the aging era, AD patients are increasing rapidly, but so far there are no fundamental treatments, but only drugs that alleviate symptoms for AD. In recent years, tau aggregates, especially tau oligomers, are known to be the main causes of memory impairment, synaptic damage, cognitive degradation, and neuronal cell death. Therefore, we have been studying the discovery of tau aggregation inhibitors as candidates for novel tau-targeted therapeutic agents. In our previous study, a high-content screening (HCS) was performed based on Tau-BiFC assay platform using FDA-approved drugs and in-house libraries, resulting in hit compound DTC0100, which is less cytotoxic and more active than Methylene Blue and LMTM, which are known as tau aggregation inhibitors in clinical study. In this study, the structural optimization of DTC0100 was carried out to generate the compound DTC2034 with improved efficacy and ADME properties, and lead optimization of DTC2034 is in progress for improving the efficacy and drug-like properties.

Poster Presentation : **MAT.P-665**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Single-layer graphene electrode significantly enhances thermoelectric property in large area molecular junction

Sohyun Park, Hyo Jae Yoon*

Department of Chemistry, Korea University, Korea

One of the main goals in organic and molecular thermoelectrics is to enhance the magnitude of thermopower. This paper describes that introducing a noncovalent interface in a molecular junction leads to a remarkable enhancement of thermopower as compared to the analogous junction with covalent interface. Thermoelectric junction measurements exhibit that the value of Seebeck coefficient in large-area junctions based on n-alkylamine monolayer on graphene is increased up to five-fold compared to the analogous junction based on n-alkanethiolate monolayer on gold. Such enhancements benefit from not only the enhanced thermal insulation arising from the noncovalent feature at the molecule-graphene interface but also reduced energy offset between transport channel and Fermi level. Our work demonstrates that control of interfacial bonding nature in molecular junctions improves Seebeck effect.

Poster Presentation : **MAT.P-666**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Fabrication of Silica Composite Nanofilms Toward Robust Antifog Nanocoating

Ji Hun Park

Department of Science Education, Ewha Womans University, Korea

Herein, I present a chemical strategy for robust antifog nanocoating with a bioinspired catalyst of silicification. Glass sponge forms its siliceous exoskeleton from a minimal concentration of silicic acid in ocean. Silicatein is the protein, isolated from glass sponge spicule, to promote diverse chemical reactions for the formation of silica structures. Inspired by the chemical knowledge of silicatein active site, cysteamine ($\text{HSCH}_2\text{CH}_2\text{NH}_2$) was suggested to be a powerful catalyst for silicification. In this context, I have supposed that the immobilization of cysteamine enables the fabrication of silica nanofilms. Due to intrinsic robustness and superhydrophilicity of silica nanofilm, the resulting silica nanofilm is believed to exhibit a long-lasting antifog effect. I combined a material-independent nanocoating strategy to immobilize cysteamine for silica composite nanocoating. The resulting silica nanofilms can resist their robustness from diverse chemical contaminations.

Poster Presentation : **MAT.P-667**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Highly reversible and stable electrochemical Ca ion insertion in a novel Ti(OH)PO₄ cathode

Richard Prabakar, Myoungho Pyo^{1,*}

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¹*Department of Printed Electronics Engineering, Suncheon National University, Korea*

The embodiment of calcium ion batteries (CIBs) is strongly limited by the sluggish Ca²⁺-ion diffusion through intercalation/de-intercalation in rigid crystalline hosts. Recent discoveries demonstrating the implementation of graphite anode in CIBs via co-intercalation of Ca²⁺ ion [1] has reignited interest among scientists to forward the CIB development by discovering new positive cathode materials capable to host Ca ions reversibly. The cathode materials candidates proposed to date suffer from many drawbacks namely, large polarization, poor cyclability, low energy storage capability, irreversible crystal structure damage, and high-temperature activation. Herein, we propose for the first time, highly reversible Ca-intercalation capability of Ti(OH)PO₄, making it a potential novel cathode material for non-aqueous CIB. Ti(OH)PO₄ (monoclinic, space group Cc) reversibly intercalates Ca²⁺ ion and displayed exceptional electrochemical cyclability and structural properties to deliver a reversible capacity of ca. 100 mAhg⁻¹ (ca. 2.6 V vs. Ca/Ca²⁺ at 0.02 mA g⁻¹ at 25°C) via a reversible transition metal ion Ti⁴⁺/Ti³⁺ redox couple reaction. Surprisingly, the structural evolution studies from ex-situ XRD studies suggested a single-phase reaction with very small topotactic volume changes during intercalation/de-intercalation, implying a robust framework. [1] S. J. Richard Prabakar, A. B. Ikhe, W. B. Park, K. C. Chung, H. Park, K. J. Kim, D. Ahn, J. S. Kwak, K. S. Sohn, M. Pyo, Adv. Sci., 6 (2019) 1902129.

Poster Presentation : **MAT.P-668**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Mutual Reinforcement between Crystal Defect Formation and Interfacial Electronic Coupling in Hybrid Electrocatalyst

Xiaoyan Jin, Seong-Ju Hwang*

Department of Materials Science and Engineering, Yonsei University, Korea

An efficient synthetic route to high-performance electrocatalysts is developed by employing conductive holey titanium nitride (TiN) nanotube (NT) with nitrogen vacancies as a hybridization matrix for Ni-Fe-layered double hydroxide (LDH). The density functional theory calculations and systematic spectroscopic analyses clearly demonstrate that there occurs an enhanced charge transfer from the surface nitrogen vacancies of holey TiN NT to Ni-Fe-LDH, leading to the feedback stabilization of nitrogen vacancies in holey TiN NT. The holey TiN-LDH nanohybrid exhibits much higher oxygen evolution reaction electrocatalytic activity and better performance for Li-O₂ batteries than do the pristine Ni-Fe-LDH and non-hole TiN-LDH nanohybrid, highlighting the beneficial role of the defective holey structure of conductive substrate. The present study underscores that the defect control of conductive hybridization matrix can provide another effective way of optimizing the electrocatalyst functionality and redox property of hybrid materials via an enhanced interfacial electronic coupling.

Poster Presentation : **MAT.P-669**

Material Chemistry

Zoom 17 FRI 15:00~16:00

TWEEN20-mediated Au–Ag long nanosnowman nanostructures with DNA-engineered conductive junction for efficient NIR photoluminescence

Jiyeon Kim, Jae-Myoung Kim, Jwa-Min Nam*

Department of Chemistry, Seoul National University, Korea

Photoluminescence (PL) from metal nanoparticles (NPs) has been considered a promising candidate for label-free sensors and imaging applications because photobleaching and photoblinking do not occur. However, it is difficult to synthesize metal NPs with a high PL quantum yield (QY), especially in the near-infrared (NIR) region which has advantages for imaging applications due to deep penetration and reduced light scattering. Therefore, developing a synthetic strategy for potent NIR photoluminescent NPs with high QY is a prerequisite for these applications. Herein, we design and synthesize TWEEN20-mediated Au–Ag head–body long nanosnowman structures (Au–Ag LNSs) from thiolated DNA-modified Au cores. The DNA-engineered conductive junction between the head and body promoted the creation of a charge transfer plasmon (CTP) mode in the NIR region. The morphology of the junction could be controlled by the DNA sequence on the Au core, resulting in thick junctions from poly thymine sequence, whereas thin junctions were formed from poly adenine sequence. We found that Au–Ag LNSs with thick conductive junctions showed higher intensities of the CTP peak and PL than thin junctions. The Au–Ag LNSs showed higher PL intensity and QY than Au nanorods with similar localized surface plasmon resonance wavelengths, and higher photostability than organic dyes, resulting in robust and sustainable PL signals under continuous laser exposure for 15 h. Finally, the PL emission from Au–Ag LNS could be detected deeper inside the scattering medium than visible fluorescent silica NPs. These results show that Au–Ag LNSs with highly strong and stable NIR PL with a high QY are promising PL nanoprobes for NIR imaging applications.

Poster Presentation : **MAT.P-670**

Material Chemistry

Zoom 17 FRI 15:00~16:00

The Synthesis of Blue-emitting $\text{In}_{1-x}\text{Ga}_x\text{P}@ZnS$ Alloy Core Quantum Dots

Yujin Kim, Seonghoon Lee*

Division of Chemistry, Seoul National University, Korea

Quantum dots (QDs) have received enormous attention as a new emitting layer due to its convenience of controlling the emitting colors and high color purity. However, widely employed ingredients, cadmium and lead, were limited to be used under the restriction of hazardous substances regulation. To develop Cd-free or Pb-free QDs, numerous researches have been conducted around the world. Among various alternatives, III-V QDs, especially indium phosphide, have gained increasing interest due to its small bulk bandgap energy (~1.34 eV) which is theoretically tunable from blue to red. However, because of its small bulk bandgap energy, the nature of III-V covalent bonding characteristic, and the lack of proper precursors, blue-emitting indium phosphide quantum dots were hard to synthesize. Here, we suggest a new method of synthesizing blue-emitting III-V-based quantum dots by introducing InGaP alloy core instead of InP core. Gallium phosphide, the same group as indium phosphide, has larger bulk bandgap energy (~2.24 eV) compared to InP. Thus, the introduction of gallium into the InP core made the core easier to have blue-emitting exciton energy. To synthesize the InGaP alloy core, new P and metal precursors with proper reactivity were required. We have produced bis(trimethylsilyl)phosphine having suitable reactivity and metal complex precursors that are soluble in the non-coordinating solvents. With new precursors, $\text{In}_{1-x}\text{Ga}_x\text{P}$ alloy core was synthesized and ZnS shell was applied onto the alloy core to increase the photoluminescence intensity. As a result, blue-emitting $\text{In}_{1-x}\text{Ga}_x\text{P}@ZnS$ QDs with high photoluminescence quantum yield and narrow full width at half-maximum (PLQY 65%, FWHM 46 nm) were successfully synthesized.

Poster Presentation : **MAT.P-671**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Acid-treated carbon nitrides as photocatalysts for RhB degradation under visible light

Suyeon Lee, Sungjin Park*

Department of Chemistry, Inha University, Korea

Carbon nitride (C_3N_4) based materials have been investigated as a photocatalyst showing high activity under visible light because of its suitable band positions. In this study, photocatalytic activity of three-dimensional (3D) melamine-derived C_3N_4 (MCN) materials was enhanced by HNO_3 activation. HNO_3 treatment under reflux removes the carbonaceous impurities in MCN and introduces oxygen-containing functional groups on its surface. Under visible light irradiation, the nitric acid treated MCN (NT-MCN) completely degrades RhB within 30 min. Photophysical characterizations and control experiments with radical scavengers reveal that MCN and NT-MCN follow different reaction mechanisms. Because NT-MCN exhibits a longer photoluminescence lifetime, smaller electrochemical resistance, and larger photocurrent than those of MCN, it enables a better transfer of charge carriers during the catalytic reaction.

Poster Presentation : **MAT.P-672**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Cell Penetrating Peptide-Modified Bumpy Au Triangular Nanoprisms for Highly Efficient Photothermal Therapy Using Low Laser Power and Low Probe Dose

Minji Ha, Jwa-Min Nam^{1,*}, Yan Lee^{2,*}

Chemistry, Seoul National University, Korea

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

²*Division of Chemistry, Seoul National University, Korea*

Photothermal therapy (PTT) exploits photo-absorbing plasmonic agents to produce heat from light, leading to subsequent tumor ablation. The main shortcomings of PTT are the side effects from inefficient heat conversion of probes, poor cell internalization, and excessive laser irradiation which can cause incomplete tumor ablation and unavoidable skin damages and affect surrounding normal cells. Hence, strong near infrared (NIR) light absorption by plasmonic probes, low-power laser irradiation, and low probe dose are important for efficient and safe PTT. Here, nanobranches were grown on Au triangular nanoprism structures to form bumpy Au triangular nanoprisms (BATrism) for increasing surface area, improving cell penetration, shifting the absorption peak to NIR region and enhancing the photothermal conversion efficiency (85.9%). Further, leucine (L)- and lysine (K)-rich cell penetrating peptides, namely LK peptides, were modified to improve cellular uptake efficiency (LK-BATrism). Significant *in vitro* therapeutic efficacy of LK-BATrism was demonstrated in human breast cancer cells under laser irradiation of very low NIR laser power (808 nm, 0.25 W/cm²). Moreover, the relatively low dose of LK-BATrism (2.5 μg Au) induced significant reduction in tumor size in mice tumor model of MDA-MB-231. Overall, this study demonstrated LK-BATrism as a promising PTT agent that enabled use of low laser power and low probe dose for realization of highly efficient and safe PTT.

Poster Presentation : **MAT.P-673**

Material Chemistry

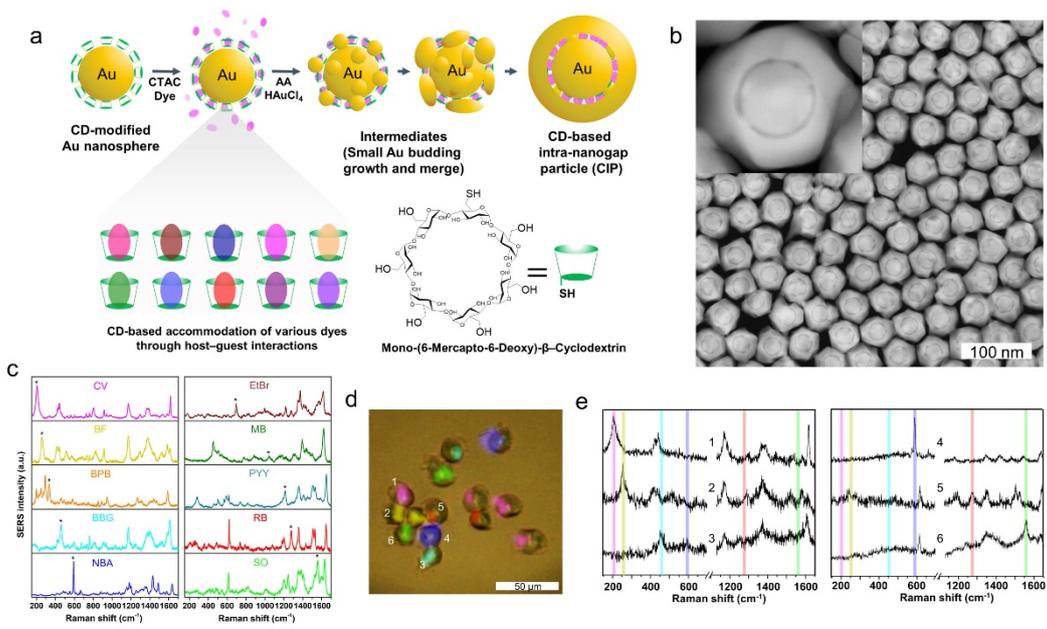
Zoom 17 FRI 15:00~16:00

Synthesis and Multiplexable Surface-Enhanced Raman Scattering Signals of Cyclodextrin-Based Plasmonic Intra-Nanogap Particles

Jae-Myoung Kim, Jiyeon Kim, Minji Ha, Jwa-Min Nam*

Department of Chemistry, Seoul National University, Korea

Plasmonic coupling between core and shell within intra-nanogap particles generates a strong electromagnetic field inside the gap, allowing for optical signal enhancements such as surface-enhanced Raman scattering (SERS). The strategy for preparing plasmonic intra-nanogap particles with well-defined nanogaps, especially around the 1 nm region, in high yields as well as positioning various Raman dyes in the gap is of paramount importance to the strong and multiplexable SERS signals. However, the preparation of highly uniform intra-nanogap particles that can accommodate various Raman dyes with a simple and facile approach remains challenging. Here, we develop a synthetic strategy to form cyclodextrin-based intra-nanogap particles (CIPs) with a well-defined ~1 nm gap by forming a gold shell on the β -cyclodextrin-modified Au nanosphere core. The cyclodextrin molecules on the core enable the formation of the uniform nanogap as well as the accommodation of various Raman dyes, generating strong and multiplexable SERS signals. The CIPs displayed the average SERS enhancement factor (EF) of 3.0×10^9 with a narrow distribution within around 1 order of magnitude ranging from 9.5×10^8 to 9.5×10^9 for ~95% of the measured CIPs. Remarkably, 10 different Raman dyes can be positioned within the nanogap of CIPs, showing 10 characteristic SERS spectra. In addition, 6 different Raman dye-loaded CIPs with little spectral overlaps were distinctly detected for cancer cell imaging applications with a single excitation source. Our strategy is a simple and facile synthetic method to form a uniform and well-defined plasmonic intra-nanogap particle with strong SERS signals and the capability of various Raman dyes accommodation through cyclodextrin molecules.



Poster Presentation : **MAT.P-674**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Synthesis of Fe₃O₄@Fluorinated SiO₂@TiO₂ Core-Shell Nano-Particles for Photo-degradation of Polyethylene

Kamran Haider

Chemistry, Sogang University, Korea

Syed Kamran Haider and Young Soo Kang* Department of Chemistry, Sogang University, 35, Baekbeomro, Mapogu, Seoul, 04107, Korea E-mail: * yskang@sogang.ac.kr Magnetite core nanoparticles were prepared by the co-precipitation method. 1 FeCl₂ (3.0 g) and FeCl₃ (6.0 g) were dissolved in 200 ml of D.I. water. 3.0 M NaOH (20 ml) and oleic acid (1.0%, v/v) were added to the solution, which changed the color of the solution from orange to black indicating the successful formation of the oleic acid-coated Fe₃O₄. Produced magnetite nanoparticles were washed by centrifugation with D.I. water and ethanol to remove NaOH and excess coating of oleic acid. The product of Fe₃O₄ nanoparticle was dried in a vacuum at 80 °C for 24 h. In the next step, fluorinated silica nanoparticles were prepared by the standard Stober process. 2 At 50 °C, ethanol and ammonium hydroxide (NH₄OH) were mixed in a beaker then a solution of TEOS ((Si(OC₂H₅)₄) was added drop by drop to the mixture solution. The transparent mixture solution turned opaque, indicating the formation of silica nanoparticles. As synthesized silica nanoparticles were fluorinated by immersing in ethanolic F3 (triethoxy[4-(trifluoromethyl)phenyl]silane) solution. Fluorinated silica nanoparticles were mixed with the oleic acid-coated magnetite particles, prepared earlier and the mixture was annealed at 300 °C to synthesize fluorinated SiO₂@TiO₂ core-shell nanoparticles to be hydrophobic on the surface. For the next step, titanium tetra-butoxide was dispersed in the ethanol, and then immediately a mixture solution of diethanolamine and water solution (1 : 1 alkoxide : water molar ratio) was dropped into it. The solution was agitated for 2 hr and then aged for furthermore 2 hr without any stirring, hence Ti sol was produced. Fe₃O₄@fluorinated SiO₂ particles were immersed into the Ti sol obtained following the stirring for 1 hr. Finally, the mixture was calcined under an airflow at 550 °C for 5 hr and Fe₃O₄@fluorinated SiO₂@TiO₂ core-shell nanoparticles were produced. TEM, TEM-EDS, HRTEM, and XRD analysis confirmed the successful synthesis of the product. Keywords: Co-precipitation, Stober process, Sol-Gel, Fe₃O₄@fluorinated SiO₂@TiO₂, Photo-degradation of

polyethyleneReferences(1) K. Petcharoen; A., Sirivat, Mat. Sci. Eng. B, 2012, 177, 421-427,(2) W. Stober;
W. Fink; A. Bohn, E. J. Colloid Interface Sci. 1968, 26, 62.



Poster Presentation : **MAT.P-675**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Enhanced Carbon Materials with Porosity and Metal Nanoparticles for Shuttle Effects

Yelim Kwon, Su Jin Kim, Ji Man Kim*

Department of Chemistry, Sungkyunkwan University, Korea

Nowadays portable electronic devices are used widely and these are indispensable part of everyday life. It makes secondary batteries important for future innovation. Li-S battery is becoming one of the promising batteries. It has high theoretical energy density and low cost. Also it is eco-friendly and safe. However, there is the primary problem to be commercialized, which is shuttle effect. It makes capacity decrease and internal resistance increase. To minimize the shuttle effect, we modified ordered mesoporous carbon(OMC) materials. OMC has high 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 due to the small pore size. In the second place, 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-676**

Material Chemistry

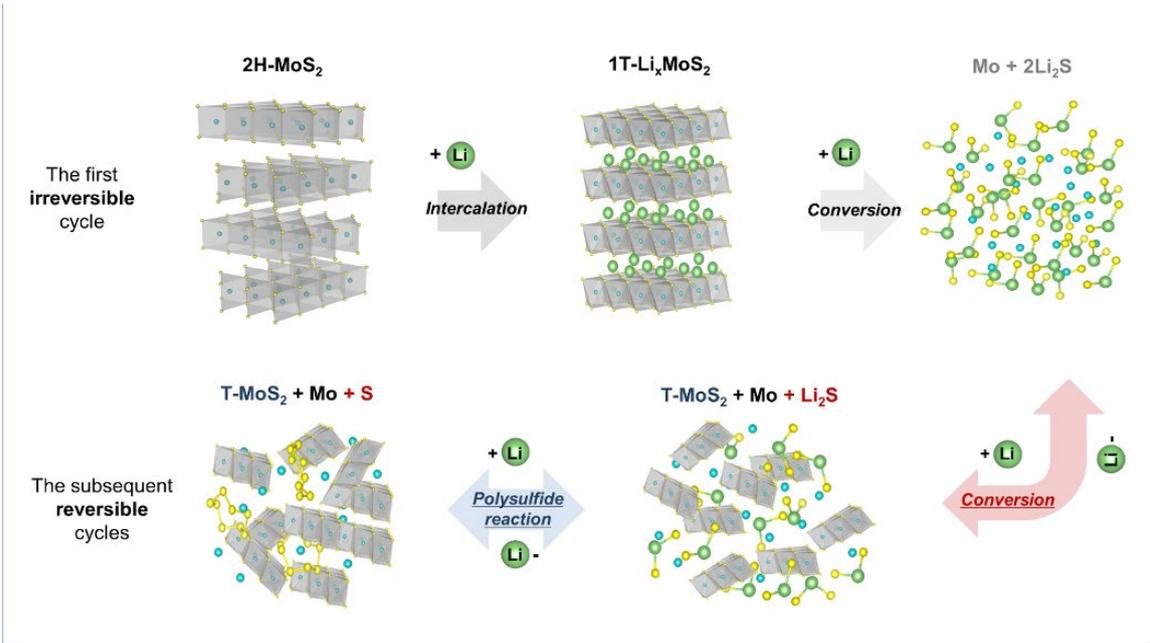
Zoom 17 FRI 15:00~16:00

Verifying Lithium Storage Behavior of MoS₂ via Synchrotron-based X-ray Analysis

Yun Seok Choi, Ji Man Kim*

Department of Chemistry, Sungkyunkwan University, Korea

Numerous studies have been conducted on a MoS₂ material owing to its high capacity and good rate capability as a promising substitute for commercial graphite materials in lithium-ion batteries. However, the mechanism of the reversible lithium-ion storage in MoS₂ remain still unclear. Herein, we carried out an in-depth study about the lithium storage behavior of MoS₂. The conversion reaction was verified by monitoring the reversible formation of MoS₂ phase through the X-ray absorption and X-ray photoelectron spectroscopies. Moreover, reversible Li-S like reactions were demonstrated by investigating the sulfur redox reaction through the voltage profile comparison and X-ray photoelectron spectroscopy deconvolution. The results of systematic approach to the reaction mechanism present clear evidence that both the Li-S like and the conversion reaction contribute to the initial obtained capacities.



Poster Presentation : **MAT.P-677**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Coexistence effects of AgBr-SnO₂-CNT nanocomposites with excellent photocatalytic activity

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The influence of coexistence effects on the microphase and the catalytic activity has gained an increased interest in recent years. For instance, combining some semiconductors with different band gaps to form heterojunctions in photocatalytic systems, because their somewhat unique properties arising from the interfacial interaction at the nanoscale were not existed in the individual nanomaterial. SnO₂, an n-type semiconductor (3.6 eV at 300 K), is being widely used in different applications due to its good acid resistance, low cost, high chemical and mechanical stability. SnO₂ has also exhibited photoactivity toward degradation of dye and other organic compounds. However, just like other transition metal oxides photocatalysts, SnO₂ suffers from low photocatalytic efficiency because of its wide bandgap and high recombination rates of photogenerated electron-hole pairs. This defects hinder the practical application of SnO₂ photocatalyst. In this study, we report a simple and effective process for coupling AgBr with SnO₂ using thiolated carbon nanotube (CNT) as an efficient photocatalyst for photodegradation of methyl orange. This study was mainly focused on: (i) optimizing a AgBr-SnO₂-CNT catalyst with high photocatalytic activity; (ii) exploring the coexistence effects of optimized AgBr-SnO₂-CNT catalyst.

Poster Presentation : **MAT.P-678**

Material Chemistry

Zoom 17 FRI 15:00~16:00

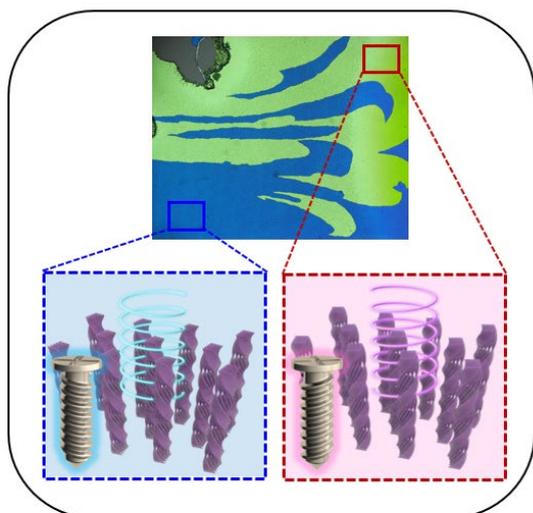
Mirror Symmetry Breaking of Helical Nanofilament by Chiral Surface

Hyewon Park, Dong Ki Yoon*

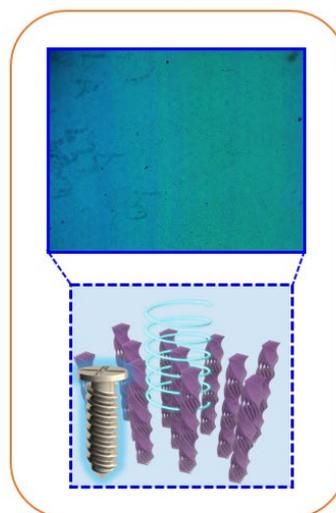
Department of Chemistry, Korea Advanced Institute of Science and Technology, Korea

The helical nanofilament (HNF or B₄) phase made of bent-shaped liquid crystal (BLC) molecules has attracted significant attention in the fields of chiral self-assembly and nano-photonics. Supramolecular chirality of HNFs is originated from the saddle-splay deformed curvature of smectic layers and show vivid structural coloration when HNFs are uniaxially aligned. However, HNFs show characteristics of the racemic mixture due to the absence of molecular chirality in BLC molecules. Until so far, despite the recent achievements, making homogenous chirality of HNFs has been a big hurdle. Herein, we present the method for controlling the chirality of HNFs based on the chiral surface and show its optical applications. We controlled the nucleation and propagation of the HNFs during the thermal phase transition, by using chiral surface and thermal gradient cooling, respectively. As a result, we successfully obtained the homochirality in HNFs whose handedness is equal to the chiral surface. Finally, a homochiral-photonic crystal was realized after uniaxial alignment of HNFs. We expect to use this film in more advanced optical applications, such as patternable color reflectors and chiral separation.

Racemic HNFs



Homochiral HNFs



Chirality
Control



Poster Presentation : **MAT.P-679**

Material Chemistry

Zoom 17 FRI 15:00~16:00

The effect of cooling rate on the structure and ion conductivity of argyrodite, solid state electrolyte material

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¹*Department of Printed Electronics Engineering, Suncheon National University, Korea*

All-Solid-State-Batteries (ASSB) are now expected to be the intrinsic solution to the problems with conventional lithium-ion batteries. In modern society, large-scale power demand and increasing energy consumption require higher safety and energy storage capabilities, which cannot be easily achieved with current state-of-the-art liquid electrolyte-based LIBs. However, the solid electrolyte to be implemented in the ASSB is expected to meet these conditions in terms of material properties. In addition, the robust nature effectively inhibits the possibility of internal short circuits and thermal runaway, significantly reducing the safety concerns of existing LIBs. Studies on solid electrolyte materials are investigated for the application of such an all-solid-state battery, the argyrodite structure materials, candidate material for solid electrolyte, is considered a promising candidate due to its high ionic conductivity. In the previously reported paper, it was confirmed that the ionic conductivity was different despite the same composition in argyrodite. These differences can occur depending on the synthesis process or measurement method. In this study, the synthesis process was changed to minimize the synthetic issue. To do this, we change cooling rate. And it was confirmed through X-ray diffraction that this phenomenon can be suppressed by controlling the cooling rate. As a result change to process, ionic conductivity was significantly increased when slow cooling process was applied. In addition, it was confirmed that the phase separation phenomenon intensifies as the amount of halogen in the structure increases.

Poster Presentation : **MAT.P-680**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Preparation and characterization of CaSnO₃-decorated carbon nanotubes for photocatalytic applications

Gyuveong Go, Hyun Chul Choi*

Department of Chemistry, Chonnam National University, Korea

Environmental problems, especially, the sustained pollutions of air and water by various organic and metallic ion contaminants receive extensive attentions. Many efforts are dedicated to the remediation of environmental pollution. Recently, it is reported that a perovskite type CaSnO₃ powders can degrade various organic pollutants under UV light irradiation. However, it is still a challenge to enhance the photocatalytic efficiency for the practical application because of the drawback of poor quantum yield caused by the fast recombination of photo-generated hole-electron pairs. In this study, we report a simple and effective process for hybridization of CaSnO₃ powders with thiolated carbon nanotube (CNT) as an efficient photocatalyst for photodegradation of ethylene blue (MB) under ultraviolet light irradiation. The prepared nanocomposite was characterized by X-ray diffraction (XRD), X-ray photoelectron spectra (XPS), and transmission electron microscopy (TEM). The prepared catalyst was found to exhibit higher photocatalytic activity than that of pure CaSnO₃.

Poster Presentation : **MAT.P-681**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Identification of molecule-based active species in Jacobsen catalyst with N-modified graphene as electrocatalysts for oxygen reduction reaction

Dawoon Jang, Sungjin Park*

Department of Chemistry, Inha University, Korea

In this study, a hybridization catalyst of Jacobsen and N-doped graphene-based materials for creating new catalytic nature was prepared as a solution process through room-temperature reaction. Jacobsen catalysts containing Co-O₂/N₂ structure are well known for converting epoxides to diols. The generation of molecularly dispersed Co-O₂/N₂-N graphene structure on the surface of graphene-based materials is confirmed by X-ray absorption, solid-state nuclear magnetic resonance, and X-ray photoelectron spectroscopic measurements. The resulting hybrid shows excellent catalytic performances for electrochemical oxygen reduction reactions (ORR). Characterizations and electrochemical measurements with control samples suggest that the Co-O₂/N₂-N-graphene structure is important for the catalytic properties. Further study with aftercycle-samples highlighted the superior stability of the active species. Theoretical calculation suggests favored ORR reactions of the fifth axial coordination of Co-O₂/N₂ by pyridinic N dopants.

Poster Presentation : **MAT.P-682**

Material Chemistry

Zoom 17 FRI 15:00~16:00

High-Performance Asymmetric Supercapacitors based on Monodisperse CuO@C Polyhedron Nanocomposites

InCheol Heo, Hyun Choi, Won Cheol Yoo^{1,*}

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Abstract Herein, CuO nanocrystals spatially embedded inside carbon polyhedron (CuO@C) derived via morphology-preserved transformation of metal-organic frameworks (MOFs) are utilized for high-performance asymmetric supercapacitors (SCs). Using a conventional MOF (several micrometers in size), pore-filling with polymer inside MOF (polymer@MOF) via vapor-phase polymerization (VPP) process was achieved that amount of polymer used for VPP can be readily adjusted to control the carbon content of CuO@C after thermolysis and subsequent oxidation processes. When monodisperse and nano-sized MOF is used for CuO@C (denoted as nCuO@C_1), it presents superior electrochemical performance because monodispersity and smaller size reduce interfacial resistance and promote mass-transport property, respectively. Asymmetric SC of nCuO@C_1 with carbon sphere (CS) as a counter electrode presents excellent energy density of 55.47 Wh/kg and long-term stability of 88.7 % at 5000 cycles, comparable to the best MO-based asymmetric SCs derived from MOFs.

Poster Presentation : **MAT.P-683**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Nanoparticle grooving with sublimable liquid crystal for anti-glare film

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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-684**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Identification of structural changes of KIT-6 synthesized with different types of alcohol

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Department of Chemistry, Sungkyunkwan University, Korea

Ordered mesoporous materials that exhibit large pore diameter, high surface area, and high pore volume have attracted enormous attention for various applications in many fields such as catalyst, adsorbent, sensors, energy storage, and nanotechnology. Among the ordered mesoporous silica, KIT-6 has 3-D cubic Ia3d structure with bi-continuous interpenetrating network, which is thought to facilitate easy access to the pore system that enables insertion and diffusion of species more efficient. According to many research, KIT-6 with various structural characteristics can be synthesized by varying synthesis parameters. Here, Structure control of KIT-6 has been done by changing the type of alcohol as a co-solvent or co-surfactant. Chain length of aliphatic alcohol was varied from C2 to C8, also considering the number and location of hydroxyl groups (-OH groups). Synthesized materials are characterized by X-ray diffraction (XRD), N₂ adsorption-desorption isotherm, and electron microscopy (SEM&TEM). Characterization results revealed that alcohol played an important role in structural formation of KIT-6. Acknowledgements : We thank to undergraduate students of Sungkyunkwan University (Hyerin Park, Jun Seok Park, Taeyeob Kim, Hyunbeom Lee, Hansol Kim, Jinyoung Myeong, Hyunju An) for experimental assistance.

Poster Presentation : **MAT.P-685**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Decellularized ECM added 3D ear cartilage scaffolds with high cell viability and biocompatibility.

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Hydrogel bio-printing technique is used in tissue engineering for artificial tissue preparation. Biocompatibility, biodegradability, printability, cytocompatibility and several mechanical properties decide hydrogel which is fit for these tissue engineering. As hydrogel, natural materials like gelatin, alginate, agarose, collagen or synthesized materials like PEG, PLA and many other materials are used to make bioink. In this study, decellularized extracellular matrix(dECM) is added to GelMA(10 % (w/v)), PEGDA(6 % (w/v)) and alginate(10 % (w/v)) mixed hydrogel in order to increase cell viability and cytocompatibility of scaffold as dECM contains components such as collagen, proteoglycan, fibronectin and laminins which increase attachment, proliferation and growth of cells. Moreover, as cells are removed from extracellular matrix to make dECM, foreign body reaction and inflammatory responses have much lower chance to occur after implantation in vivo. Using this dECM added scaffold, we can make not only ear cartilage scaffold but also diverse scaffolds that are applicable in human body. Also, basic physical and mechanical properties, and cell viability of dECM added hydrogel are studied in this research.

Poster Presentation : **MAT.P-686**

Material Chemistry

Zoom 17 FRI 15:00~16:00

Study on optical properties of Yb³⁺, Er³⁺, and Eu³⁺ -codoped Sr₂YF₇

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Upconversion fluorescence is the process of converting optical energy from low absorption energies to high emission energies. The upconversion materials exhibit significant advantages such as high penetration depth, low unwanted autofluorescence, and light scattering from biological species at near-infrared excitation. In this work, we present the optical properties of Yb³⁺, Er³⁺, and Eu³⁺ -codoped Sr₂YF₇. The material was synthesized by a co-precipitate method and exhibited strong upconversion emission and downconversion under 980 nm, and UV excitation wavelength respectively. The upconversion process originated from Yb³⁺-Er³⁺ ion pairs, whereas downconversion is related to Eu³⁺ ions. The performance of color emission of the prepared material was estimated using the Commission International de l'Eclairage (CIE) chromaticity coordinates.

Poster Presentation : **MAT.P-687**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Strong Mid-IR Emitter, Tellurium Element and Microcrystals

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Tellurium is a semiconductor with a narrow bandgap (0.33 eV) and the fourth most abundant element in the human body. Many researches have been reported the physical properties of Te crystal because of the high thermoelectric property and photoconductivity. Also, various morphologies of Te crystals were studied such as nanorods, nanowires, nanotubes, 2-D tellurene, and chiral nanostructures. Nevertheless, the photoluminescence (PL) at room temperature has never been reported. Here, we present the room-temperature PL ($\sim 2670\text{ cm}^{-1}$) of tellurium elemental solid and microcrystals. When lowering the temperature or increasing the pump fluence, the random lasing was achieved in the bulk Te crystal and whispering gallery mode was operated in the rod-shaped microcrystals. Second-harmonic generation (SHG) and third-harmonic generation (THG) were shown for the rod-shaped microcrystals. MWIR lasing property and the strong PL emission intensity of the Te element and microcrystals will be used as a great mid-IR emitter and provide new applications in optoelectronics, etc.

Poster Presentation : **MAT.P-688**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Mineralization of Indigo Carmine under Visible light Using ZnBi₂O₄-Bi₂S₃ Composites

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¹*Department of Chemistry, Changwon National University, Korea*

Novel highly visible-light active ZnBi₂O₄-Bi₂S₃ photocatalysts have been synthesized by a simple two-step co-precipitation and hydrothermal method. The efficiency of the prepared ZnBi₂O₄-Bi₂S₃ composites was evaluated for the degradation of Indigo carmine in aqueous solutions under visible light irradiation. The photocatalytic activities of the prepared ZnBi₂O₄-Bi₂S₃ composites was higher than that of pristine ZnBi₂O₄. This enhancement could be attributed to synergetic effects, charge transfer between ZnBi₂O₄ and Bi₂S₃, as well as the separation efficiency of the photogenerated electrons and holes. These results demonstrate the feasibility of utilizing ZnBi₂O₄-Bi₂S₃ as potential heterogeneous photocatalysts for environmental remediation.

Poster Presentation : **MAT.P-689**

Material Chemistry

Zoom 17 FRI 16:00~17:00

New Formulation of Silver Reactive Ink Compatible with Macroporous Paper Substrates for the Development of Paper-based Electronic Device

Sharipov Mirkomil, Yong-Il Lee*

Department of Chemistry, Changwon National University, Korea

The reactive ink composed of a silver-organic complex has shown the ability to generate silver cations which are further reduced into highly conductive silver metal nanoparticles on various substrates such as glass and PET. However, the incompatibility with a Whatman No.1 and conventional office paper, on which silver cations transduces to silver oxides and revert to silver complex, has limited its application in developing flexible paper-based electroanalytical devices such as electrofluidics and microfluidics devices. In this work, polyvinylpyrrolidone (PVP) was introduced as a stabilizing agent of silver cations generated from the decomposition of silver-reactive ink on hydroxyethyl cellulose (HEC)-premodified Whatman No.1 paper to enable the formation of silver metal nanoparticles. FTIR studies confirmed the stabilization of silver cations by PVP through nitrogen and oxygen atoms. TGA results have confirmed that the combination of PVP and HEC-modified paper allows decreasing the curing temperature to 60 °C by limiting the formation of silver acetate complex and silver oxides. Moreover, XRD patterns confirmed the formation of silver metal nanoparticles resulting in a high conductivity on microporous paper, calculated to be $6.246 \times 10^6 \text{ S m}^{-1}$. FE-SEM images confirmed the uniform distribution of silver nanoparticles exclusively on the surface of the cellulose fibers simultaneously preserving the porosity of paper. The microporous silver patterned paper was further coated with a ferroelectric fluoropolymer: PVDF-HFP to enhance its electrowetting properties and was applied in the development of a paper-based microfluidic device equipped with an electrical valve.

Poster Presentation : **MAT.P-690**

Material Chemistry

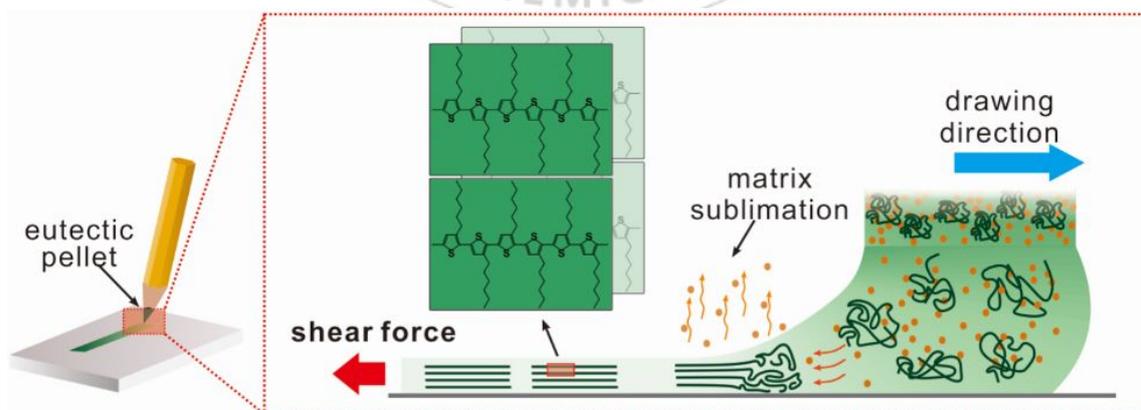
Zoom 17 FRI 16:00~17:00

Uniaxially Aligned Semiconducting Polymers by Using Eutectic Friction Transfer Lithography

SangWon Eom, Youngjong Kang*

Department of Chemistry, Hanyang University, Korea

As the usage of semiconducting polymers is increased, various polymer alignment techniques are developed to improve their electrical and optical properties. But their sophisticated condition and equipment limit to draw various pattern or combine with other techniques. Therefore, simple and convenient techniques which can make various pattern easily and be compatible with other techniques are needed. So, we report a solid-state lithography technique utilizing the eutectic friction transfer (EFT). Eutectic friction transfer lithography (EFTL) technique employs the eutectic pellets made of semiconducting polymers and volatile organic solid matrixes. With utilizing frictional heating and eutectic melting, various semiconducting polymer crystals formed by simple rubbing process at mild condition. Strong anisotropic optical properties suggest that J-type packing is dominant in EFTL microwires because of the highly extended and planarized crystal structures.



Poster Presentation : **MAT.P-691**

Material Chemistry

Zoom 17 FRI 16:00~17:00

MOFs-Derived Carbon Mediated Interfacial Reaction for the Synthesis of CeO₂-MnO₂ Catalysts

Lianghao Song, Ji Man Kim*

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CeO₂-based catalysts are widely studied in the catalysis fields. Developing one novel synthetic approach to increase the intimate contact between CeO₂ and secondary species is of particular importance for enhancing catalytic activities. Herein, we design an interfacial reaction between MOF-derived Carbon and KMnO₄ to synthesize CeO₂-MnO₂, 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 CeO₂ crystallites at high calcination temperature, and more importantly, the intimate contact within CeO₂/C is conveyed to CeO₂/MnO₂ after interfacial reaction, which are responsible for high catalytic activity of CeO₂-MnO₂ towards CO oxidation.

Poster Presentation : **MAT.P-692**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Anisotropic 2D-SiAs nanosheet for High-Performance UV-Visible Photodetectors

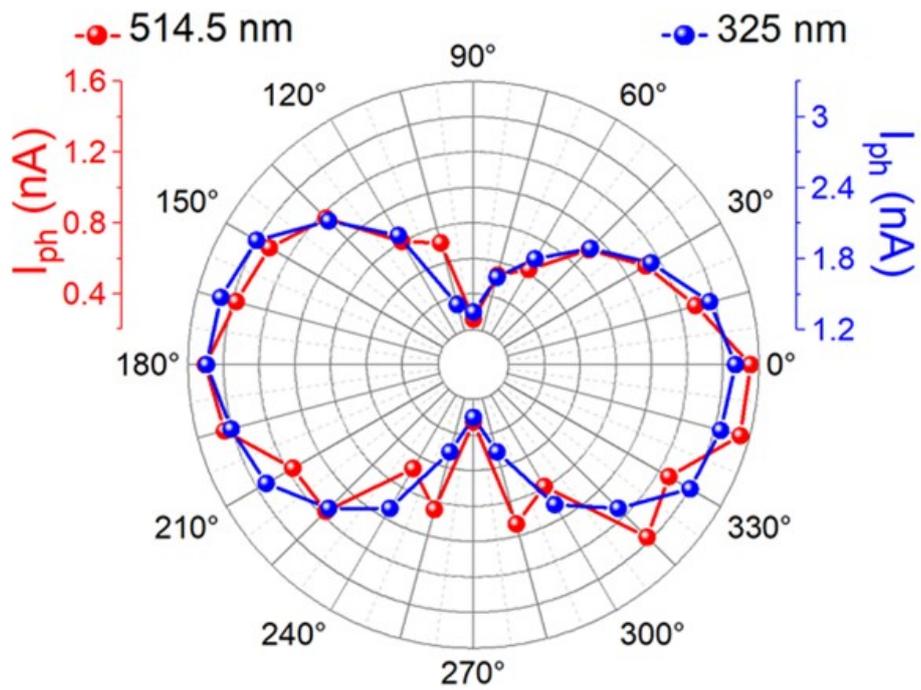
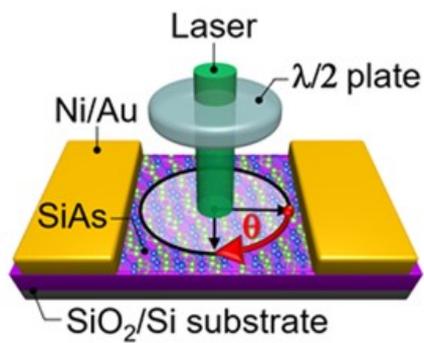
Doyeon Kim, In Hye Kwak¹, Ik Seon Kwon, Jeunghee Park^{2,*}

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We report the in-plane anisotropic optical and (photo)electrical properties of SiAs nanosheets synthesized using a baking sealed quartz tube method and subsequent mechanical exfoliation. The angle-resolved polarized Raman spectrum shows high in-plane anisotropy of the phonon vibration modes, which are consistent with the theoretical prediction. Field-effect transistor devices fabricated using the SiAs nanosheets demonstrated significant anisotropy in the hole mobility with an anisotropic ratio as high as 5.5. Photodetectors fabricated with single SiAs nanosheet exhibited high sensitivity in the UV-visible region, and the anisotropic ratio of the photocurrent reached 5.3 at 514.5 nm and 2.3 at 325 nm. This work lays the foundation for future research in anisotropic 2D materials.



Poster Presentation : **MAT.P-693**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Structural Design and Custom Application Induced by Multi-Combined Guest Molecules in Metal-Organic Frameworks

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Organic molecules have excellent reactivity and selectivity and are used in various fields such as catalyst, energy conversion devices, sensors, chemical reaction, fluorescent dye, and etc. However, due to the organic molecular structure, there is a limitation of structural instability such as intermolecular dimer reaction and self-quenching in solution. To overcome these limitations, studies have been conducted to improve stability by adding special functional groups to organic molecules or attaching them to the surface of inorganic support. However, it takes a lot of time and cost to transform and synthesize the large complicated molecular structure for a specific application. In this study, it is provided a tailored platform suitable for each application while maintaining the unique properties of the widely used photoactive molecules. Therefore, the spatial design based on the metal-organic frameworks (MOFs), which is a porous structure, was studied to improve platform-based characteristics and impart functions, not the structural modification of the molecule itself. The MOF is a structure formed by self-assembly of metal clusters and organic ligands, and has a porous crystalline structure in which pores are regularly arranged. By utilizing these advantages of MOF, which enables structural design and has excellent space utilization performance, it accesses three spaces, the inner pores, the structural skeleton, and the outer surface, to improve the stability of organic molecules and optimize performance accordingly. Therefore, this study deals with research applied to rhenium complex photocatalyst and fluorescent bio-imaging agent with targeting properties by custom designing organic ligands constituting the skeleton of the MOFs and pores constituting the interior.

Poster Presentation : **MAT.P-694**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Pomegranate- like Fe₃O₄ Nanocrystal Assembly in a 2D-wrinkled Porous Carbon Material for High Power Density Pseudocapacitor

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¹Department of Chemistry, Sogang University, Korea

Since ancient times, onwards carbon-based materials play a copious role in almost every aspect of human civilization, including the energy field. However, the copious development of industries and depletion of fossil fuels generate deteriorating environmental pollution and an appalling economic crisis. Thus, there are increasingly necessary for developing well-defined nanostructures to mitigate energy and environmental issues. Herein, we present a unique concerted method to convert agro bio-waste into an economical wealth material. By the inspiration of nature, we selected a waste 2D garlic husk (*Allium sativum*) as a torchbearer to make a unique material. Moreover, by considering the fascinating properties like high surface area conjugated hexagonal network, chemically more reactive edge sites, durable mechanical strength, open van der Waals gaps, and unique flexible atomic dimensions allow 2D carbon materials are a key component for energy storage and production. The garlic extract was applied for the synthesis of Fe₃O₄ nano-assemblies (NAs) embedded in 2D-CCS composite. Interestingly, the small-sized Fe₃O₄ nanocrystals (⁻¹), and ultra-high power density (3500–8000 W kg⁻¹) for pseudocapacitor application, which is one of the best materials among the Fe₃O₄ based electrode materials. This simple work stimulates a new door for the generation of waste to well-defined nanostructure materials for energy, catalysis, and environmental applications



Poster Presentation : **MAT.P-695**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Post-synthetic Incorporation of Trivalent Gallium ion into Layered Double Hydroxide Lattice through Dissolution-Reprecipitation at the Edge and Isomorphous Substitution in the Core

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Trivalent gallium ion was successfully incorporated into the chemically well-defined MgAl-layered double hydroxide (LDH) frameworks through post-synthetic hydrothermal treatment. In order to reduce the acidity of trivalent metal, $\text{Ga}^{3+}(\text{aq})$ was pretreated with NaOH to produce $\text{Ga}(\text{OH})_4^{-}(\text{aq})$, which was reacted with LDH suspension under hydrothermal condition at 150°C. Quantitative analysis using inductively coupled plasma-mass spectroscopy showed that Ga^{3+} was first incorporated into LDH through partial dissolution-precipitation at the edge of LDH particles and was then uniformly distributed throughout the particle by substitution of Ga^{3+} for Al^{3+} in LDH frameworks. The molar fraction of Ga^{3+} in the LDH framework gradually increased from 0% to 2.6% along the reaction time from 0 h to 24 h. The powder X-ray diffraction patterns showed that the Ga^{3+} incorporation did not influence the crystal structure without the evolution of impurities such as GaOOH . The morphology and surface property of LDH, confirmed by scanning electron microscopy and dynamic light scattering, suggested the preservation of physicochemical properties during 24 h of hydrothermal reaction. The distribution of incorporated Ga^{3+} was investigated with energy dispersive spectroscopy-assisted transmission electron microscopy, visualizing the homogeneous location of Ga^{3+} in an LDH particle. The X-ray absorption near-edge structure and extended X-ray absorption fine structure exhibited that the Ga moiety was stably incorporated in the LDH lattice from 0.5 h and gradually crystallized with reaction time (~ 24 h).

Poster Presentation : **MAT.P-696**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Highly increased stability of L-ascorbic acid by hybridization with inorganic layered yttrium hydroxide

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Layered yttrium hydroxide (LYH), a member of the layered rare earth hydroxide family, was prepared by the coprecipitation method in hexamethylenetetramine (HMT) solution. L-ascorbic acid was then successfully hybridized into the galleries of LYH by typical anion-exchange reaction in an aqueous solution. Variation in XRD patterns accompanied with host-guest reaction suggested a bilayer arrangement of ascorbate anions in the interlayer space of LYH, which is different from a single layer arrangement in the classical layered double hydroxides (LDHs). The difference in anion-exchange capacity and layer charge density between LDH and LYH would result in such a different arrange fashion of ascorbate anions in corresponding interlayer gallery. Because the $M2+/M3+$ ratio is limited for the brucite-type layer structure of LDHs, LYH is expected to have the higher charge density and consequently the higher anion-exchange capacity. It is also expected that the interlayer anions interact more strongly with hydroxide layers of higher positive charge density. Based on thermogravimetric analysis results, the loading ratio of ascorbate in LYH was close to ~95% of its maximum ion-exchange capacity, which was much higher than ~ 84 % in Zn-Al LDH. FT-IR and UV-vis absorption spectroscopic analysis revealed that the formation of ascorbate-LYH hybrid system substantially enhanced the stability of L-ascorbic acid against photo as well as oxidative degradation. Therefore, LYH is proposed as a good host material for both safe storage and delivery of L-ascorbic acid.

Poster Presentation : **MAT.P-697**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Improvement of thermoelectric effect by fabrication of nanocomposite grain boundary via a cation exchange

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Eco-friendly coated grain nanocomposite was synthesized by cation exchange of nanoparticle surface. Coating layer of CuInTe₂ was formed at the grain boundary of SnTe. Copper acetate and indium acetate were selected as cation precursors for cation exchange by considering thermodynamic and kinetic factors. CuInTe₂ has negative formation energy and lower solubility product, therefore, CuInTe₂ could be precipitated spontaneously. The acetate as a ligand of ingoing cation was used considering Pearson's hard and soft acids and bases concept. Soft acids Cu²⁺ and In³⁺ can be released from a hard acetate base and they are participated via cation exchange reaction and acetate ligands induce a hard acid Sn²⁺ to be dissolved out from the surface of particles to form tin acetate which is a stable acid-base pair. From a kinetic perspective, we considered crystal structure similarities of surface coating layer and SnTe particles. The coating layer of CuInTe₂ has the same Te arrangement as that in SnTe however, cations of Cu⁺ and In³⁺ are occupied in tetrahedral sites. Consequently, coating layer of CuInTe₂ were formed via a cation exchange of Sn²⁺ in octahedral sites by Cu⁺ and In³⁺ in tetrahedral sites. The coating layers were contributed as a potential barrier and phonon scatterer. Therefore, it enhanced the Seebeck coefficient by 40% through carrier energy filtering and reduced the lattice thermal conductivity by about 50% by coherent phonon scattering. The thermoelectric figure of merit (zT) in this eco-friendly nanocomposite composed of CuInTe₂ coated grain boundaries in SnTe was 1.68 at 823K and this value is an approximately 170% improvement value over uncoated SnTe. Also, the average zT value at 373~ 823K range was 0.76 and it is expected to be utilized in the industrial application.

Poster Presentation : **MAT.P-698**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Understanding Structure-Property Relations in Perovskite Light-Emitting Diodes via Interfacial Engineering with Self-Assembled Monolayers

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Department of Chemistry, Korea University, Korea

In the research of perovskite light emitting diodes (PeLEDs), reliable understanding on structure-property relations is necessary, yet singling out one effect from others is difficult since photophysical and electronic functions of PeLEDs are interwoven each other. This presentation reports on the role of self-assembled monolayers (SAMs) for interfacial engineering nanomaterials in the performance of PeLED. Four different molecules that have the same anchor (thiol), different backbone (aryl vs. alkyl) and different terminal group (amine vs. pyridine vs. methyl) are used to form SAMs at the interface with the thin film of green-color perovskite, $\text{CH}_3\text{NH}_3\text{PbBr}_3$. Experiments reveal how the chemical structure of molecule comprising SAM is related to the various chemical and physical features such as quality and grain size, cross-sectional atomic composition (Pd(0) vs. Pd(II)), charge carrier lifetime, charge mobility of perovskite films. The trends observed in the model system stem from the affinity of SAM over the undercoordinated Pb ions of perovskite, and these are translated into considerably enhanced EQE (from 2.20 to 5.74%) and narrowband (from 21.3 to 15.9 nm) performances, without noticeable wavelength shift in PeLEDs. Our work demonstrates that SAM-based interfacial engineering holds a promise for not only deciphering mechanisms of perovskite LEDs but also improving the device performance.

Poster Presentation : **MAT.P-699**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Transparent and Flexible AuNPs Cellophane Surface Enhanced Raman Scattering (SERS) Sensors Synthesized by Dry Plasma Reduction Method

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In this study, we demonstrate the synthesis method of a transparent and flexible surface-enhanced raman scattering (SERS) substrates composed of Au nanoparticles (AuNPs) and cellophane. AuNPs were simply synthesized on the cellophane substrate from reduction reaction of Au³⁺ ions by using Ar dry plasma without adding any chemical. The density of AuNPs formed on the cellophane substrate was controlled with the concentration of Au³⁺ precursor ions. The SERS activity was affected by the electromagnetic enhanced on the hotspot between the small gaps of AuNPs on the substrate. The AuNPs cellophane substrate detected benzethiol as raman probe with high enhancement factor (EF) value (~5.5 x 10⁶). Moreover, it is possible to measure raman signal on both sides of the substrate due to its transparent characteristic. It shows possibility applying for direct detection of pesticide by attaching at food such as fish and fruit.

Poster Presentation : **MAT.P-700**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Fe intercalation of VSe₂ Nanosheets by Solvothermal Reaction

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¹*Micro Device Engineering / Microdevices, Korea University, Korea*

Group V (e.g., V, Nb, and Ta) transition metal dichalcogenide (TMD) had emerged as another promising 2D materials, but the related research has been behind that of Group VI TMDs (e.g., MoS₂, WS₂). They belong to the metallic TMD family with no band gap in electronic states and exhibit strong dimensionality effects in their unique properties such as superconductivity, ferromagnetism, and charge-density wave transition. Moreover, their van der Waals interlayers contain either octahedral or trigonal-prismatic vacancies, which provides intercalation sites for a diverse range of intercalated metal atoms including the native atoms that present in the TMD itself. Herein, we synthesized Fe-intercalated VSe₂ (Fe_xVSe₂) nanosheets with a controlled composition of x = 0-0.5 using a solvothermal reaction. The Fe intercalation induced unique phase evolution from 1T VSe₂ to 1T' phase after x = 0.25. The electronic structure analysis revealed the higher oxidation states of V and Fe as the x increases. The superparamagnetic properties at room temperature reach a maximum at x = 0.3, supporting the octahedrally coordinated Fe atoms. First-principles calculation was performed for the intercalation models that show distinctive phase transition at various Fe composition.

Poster Presentation : **MAT.P-701**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Mo_{1-x}V_xSe₂ Alloy Nanosheets with Rich Dual V/Se Vacancies and Their Excellent Catalytic Activity Toward Hydrogen Evolution Reaction

In Hye Kwak, Ik Seon Kwon¹, Seungjae Lee¹, Doyeon Kim¹, Jeunghye Park^{2,*}

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²*Department of Materials Chemistry, Korea University, Korea*

Two-dimensional transition metal dichalcogenide has attracted much attention due to their excellent electrocatalytic performance for the hydrogen evolution reaction (HER). Herein, we report a solvothermal synthesis of composition-tuned Mo_{1-x}V_xSe₂ alloy nanosheets over whole range. Alloying results in a phase transition from semiconducting 2H phase MoSe₂ to metallic 1T phase VSe₂ at x = 0.5-0.6. Detailed structure analysis including atomically resolved scanning transmission microscopy revealed that the VSe₂ tend to aggregate in atomic scale and prefer the metal/Se vacancies. They exhibit excellent electrocatalytic HER performance at x = 0.2-0.3 in 0.5 M H₂SO₄ and 1 M KOH with a current of 10 mA cm⁻² at an overpotential of 110 and 160 mV (vs. RHE) and a Tafel slope of 43 and 76 mV dec⁻¹, respectively. Our extensive spin-polarized density function theory calculations predicted the phase transition at x = 0.5-0.6 consistently with the experimental results. Calculation of the formation energy for Se/metal vacancies showed that alloying produced more significant vacancies compared to MoSe₂ and VSe₂. The VSe₂ domain favors the formation of V and Se vacancies in an aggregated way. The Gibbs free energy along the reaction path indicates that the best HER performance originated from the highest concentration of active sites that form V-H in the Se vacancies.

Poster Presentation : **MAT.P-702**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Concurrent Vacancy and Adatom Defects of $\text{Mo}_{1-x}\text{Nb}_x\text{Se}_2$ Alloy Nanosheets Enhanced Electrochemical Performance of Hydrogen Evolution Reaction

Ik Seon Kwon, In Hye Kwak¹, Seungjae Lee, Doyeon Kim, Jeunghye Park*

Advanced Materials Chemistry, Korea University, Korea

¹*Micro Device Engineering / Microdevices, Korea University, Korea*

Earth-abundant transition metal dichalcogenide nanosheets have emerged as an excellent catalyst for electrochemical water splitting to generate H_2 . Alloying the nanosheets with heteroatoms is a promising strategy to enhance their catalytic performance. Herein, we synthesized hexagonal (2H) phase $\text{Mo}_{1-x}\text{Nb}_x\text{Se}_2$ nanosheets over the whole composition range using a solvothermal reaction. Alloying results in a variety of atomic-scale crystal defects such as Se vacancies, metal vacancies, and adatoms. The defect content is maximized when x approaches 0.5. Detailed structure analysis revealed that the NbSe_2 bonding structures in the alloy phase are more disordered than the MoSe_2 ones. Compared to MoSe_2 and NbSe_2 , $\text{Mo}_{0.5}\text{Nb}_{0.5}\text{Se}_2$ ($x = 0.5$) exhibits much higher electrocatalytic performance for hydrogen evolution reaction. First-principles calculation was performed for the formation energy in the models for vacancies and adatoms, supporting that the alloy phase has more defects than either NbSe_2 or MoSe_2 . The calculation predicted that the separated NbSe_2 domain at $x = 0.5$ favors the concurrent formation of Nb/Se vacancies and adatoms in a highly cooperative way. Moreover, the Gibbs free energy along the reaction path suggests that the enhanced HER performance of alloy nanosheets originates from the higher concentration of defects that favor H atom adsorption.

Poster Presentation : **MAT.P-703**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Engineering of Biomimetic Hybrid Extracellular Matrix for Tissue Regeneration

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Extracellular matrix is a connective fiber network supporting cells living in its surrounding environment. Particularly, in basal region of skin tissue, a multi-component extracellular matrix, mainly composed of fibronectin (FN), laminin (LN) and collagen (COL) are formed in forms of fibers. They are organized in distinct architecture and specific composition of each tissue. In tissue, cells are aligned in one direction on their natural ECM network. In this study, we generated a controllable orientation and multi-component of ECM network. Here, we harnessed fibrillogenesis to mimic cellular ECM on ECM components micropattern, mainly FN. We simultaneously and subsequently manipulated the ECM components network by micropatterning various ECM molecules (FN, LN and COL) to control architecture cellular ECM synthesis. We found that the cellular FN network undergoes fibrillogenesis on the ECM components micropattern. When external FN was added to the systems, it unfolded and extended FN fibril formation, which clearly confirmed by fluorescence resonance energy transfer (FRET) assay. Thus, fibril form of external FN bound to cellular FN in order to form a hybrid FN network. Added COL and LN also could build a distinct ECM network to the system. Therefore, we believe that this study could provide a controllable multi-component ECM network fabrication as a novel platform for cell-mimicking ECMs in tissue engineering. Keywords: extracellular matrix, fibronectin, laminin, collagen, FRET

Poster Presentation : **MAT.P-704**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Hybrid Membrane Catalyst of Porous-Layered Double Hydroxide and Dense Gold Nanoparticles

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We have synthesized the hybrid catalyst of porous-layered double hydroxide (LDH) decorated with dense gold nanoparticles. The porous LDH was prepared using a coprecipitation and aqueous miscible organic solvent treatment (AMOST) method, resulting in thin LDH platelets. Following spray dry produced the porous LDH like a hydrangea structure providing an extensive open network with a 300 m²/g of BET surface area. Its large open structure and active hydroxide surface have enabled uniform decoration of an average 10 nm diameter of gold catalysts by one-pot chemical reduction using NaBH₄ at room temperature. Due to a few hundred nm of porous LDH, filtration of the hybrid colloid solution gave a membrane catalyst, potentially useful in continuous catalytic reactions, e. g. hydrogenation of p-nitrophenol. This study suggested that their porous structure and active gold nanocatalyst allowed fast and mass catalytic functions by the simple filtration process. We found no significant damage to the hybrid membrane during a few liters of reactions, expecting strong bindings of the gold nanoparticles on the porous LDH.

Poster Presentation : **MAT.P-705**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Intra and Intermolecular Charge Transfer Control by Electron Push-Pull Substitution: Mechanofluorochromism Tuning

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A series of symmetrical, planar 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 the electron push-pull substituent effect on the photophysical and mechanofluorochromic (MFC) properties. An examination of the photophysical and electrochemical properties of **CN-OMe** revealed a gradually regulated energy bandgap consistent with the substituent effect as it progressed from an electron-withdrawing group (EWG) to an electron-donating group (EDG). In particular, the Lippert-Mataga equation showed that the electron push-pull substituent effect controlled the energy levels of two different excited states. Despite the D-A-D system, **CN** emission originated only from the locally excited (LE) state. Femtosecond transient absorption measurements showed a gradual transition from the LE state to the intramolecular charge transfer (ICT) state according to the substituent effect and no transition from the LE to ICT state for **CN**. Interestingly, Py 2,7-positions D-A-D based MFC phenomena were observed and showed electron push-pull substituent effect dependent MFC behavior. This study suggests that as the EWG ability increases, the intramolecular interactions become insufficient and induce strong intermolecular D-A interactions for stabilizing molecules, leading to high MFC efficiency that are reversibly repeated several times.

Poster Presentation : **MAT.P-706**

Material Chemistry

Zoom 17 FRI 16:00~17:00

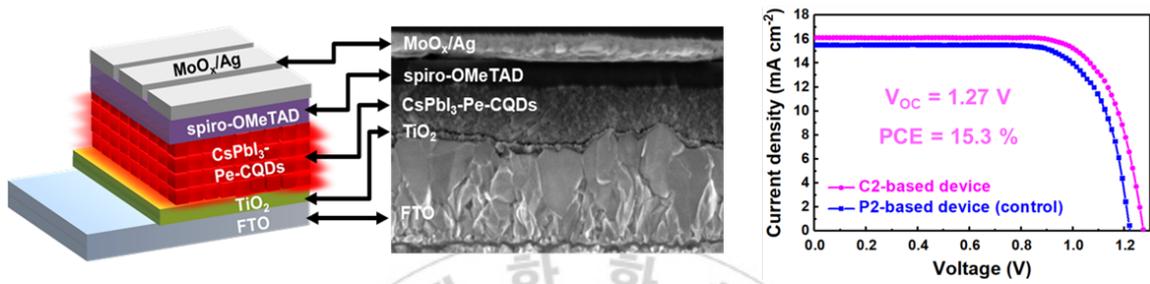
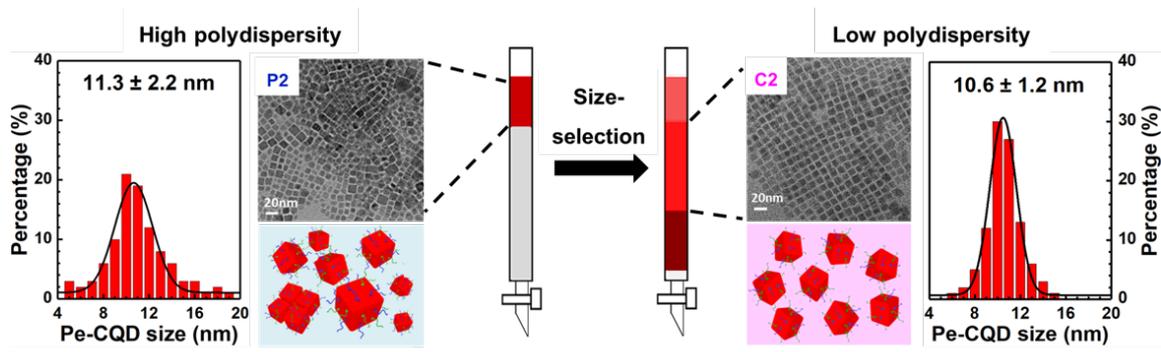
Development of High-Efficiency Perovskite Colloidal Quantum Dot Solar Cells via Increasing Monodispersity

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Bandtail broadening in inhomogeneous colloidal quantum dots (CQDs) result in losses in open-circuit voltage (Voc) and inhibited carrier transport in photovoltaics. For perovskite CQDs (Pe-CQDs), which are recently employed as a promising photovoltaic absorber, bandtails are broadened by Pe-CQD polydispersity and inhomogeneous agglomeration during the purification process. Although the monodisperse Pe-CQDs is highly required for further improving the device performance in the solar cells, no studies have been reported on the relationship between the polydispersity and device performance of Pe-CQD solar cells thus far. Herein, we report for the first time that the photovoltaic performance of solar cells based on the fully-inorganic CsPbI₃-Pe-CQDs can be improved by reducing the energetic disorder with bandtail sharpening, achieved using the monodisperse Pe-CQDs with low polydispersity. Size-selection process based on the gel permeation chromatography (GPC) method is employed to effectively remove the large and small particles in the purified Pe-CQDs, thereby enabling the preparation of the monodisperse Pe-CQDs showing the high photoluminescence (PL) quantum yield, narrow PL full-width at half maximum (FWHM), and low Urbach Energy. These monodisperse Pe-CQDs result in enhancing the light absorption by the reduction in the energetic disorder with bandtail sharpening below the optimum bandgap. Thanks to these advantages, monodisperse Pe-CQDs improve the photovoltaic performance of solar cells up to 15.3% PCE with a Voc of 1.27 V, which are the highest PCE and Voc among the single-composition CsPbI₃-Pe-CQD solar cells reported so far.



Poster Presentation : **MAT.P-707**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Electronically Tunable and Thermally Activated Delayed Fluorescence: Click-To-Twist Strategy To Build Donor–Acceptor-type Emitters

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Department of Chemistry, Seoul National University, Korea

Invention of a new chemical moiety is the foundation to create efficient materials. For thermally activated delayed fluorescence (TADF) emitters that operate by intramolecular charge-transfer (ICT), donor, acceptor, and π -spacer are the key structural components. In this presentation, we disclose a “click-to-twist” strategy to build a new 1,2,3-triazole-based acceptor unit, and its applications to blue-to-green TADF emitters. Our synthetic strategies allowed systematic modulation of the electronic and steric properties to control excited-state photophysics. Six different emitters were prepared in a modular fashion by varying the donor strength and π -spacer steric factors for mix-and-match. The materials display deep blue to sky blue emission, and TADF properties in both solution and doped film samples. Organic light-emitting diode (OLED) devices fabricated with these materials exhibit high external quantum efficiencies of up to 20.7%, and maximum luminance of 6823 nit. Building upon a straightforward and intuitive method to construct sterically congested aryl-rich molecules, this work represents a new strategy to make TADF emitters by mechanism-based design and modular synthesis.

Poster Presentation : **MAT.P-708**

Material Chemistry

Zoom 17 FRI 16:00~17:00

Triazine-dibenzofuran based n-type host material for high efficiency and long lifetime in green phosphorescent organic light-emitting diodes

Sunhee Lee, Won-Sik Han*

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A series of triazine-dibenzofuran-based n-type host materials, **DBT1–DBT4**, were prepared by varying the substitution position of dibenzofuran to study their structure-property relationships on photophysical, thermal, and electrochemical properties along with device performances. The results demonstrated that the substitution position of dibenzofuran significantly affects the chemical structure which results different electrochemical and photophysical properties. All developed materials were utilized in green phosphorescent organic light-emitting diodes (PhOLEDs) as a n-type host material mixed with p-type host (**BPCz**) in the mixed host. To assess the electroluminescence (EL) properties of these n-type host materials, 16 devices were fabricated and systematically analyzed. Among them, the green PhOLEDs using **DBT4/BPCz** display the best EL performances with high current efficiency up to 131.98 cd A⁻¹, external quantum efficiency up to 30.90%, and power efficiency up to 105.44 lm W⁻¹ with device lifetime (T₉₅) for 180 hours at 10,000 nits.

Poster Presentation : **MAT.P-709**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Nobel synthesis of porous carbon-supported molybdenum nitride oxidative desulfurization catalyst from phosphomolybdic acid loaded metal-azolate framework-6

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Removal of thiophenics from crude liquid fuel is important for our sustainability, and oxidative desulfurization (ODS) is one of the promising methods when a highly active catalyst is available. In this study, a new composite of the metal-azolate framework (MAF-6) and phosphomolybdic acid (PMA), named PMA(x)@MAF-6, was prepared via in-situ synthesis method. Well-dispersed (size: ~4 nm) molybdenum nitride (Mo₂N), on highly porous carbon, was prepared firstly via high-temperature carbonization of the PMA(x)@MAF-6 composite. The prepared catalyst was applied in ODS, in the presence of hydrogen peroxide (H₂O₂) as a green oxidant and showed remarkable performance. A selected catalyst Mo₂N@C-3 had the high turnover frequency (TOF, 30 h⁻¹) with the lowest activation energy (27.8 KJ·mole⁻¹) in ODS (with H₂O₂). The oxidation of thiophenics over Mo₂N@C was explained by a non-radical mechanism via active Mo-peroxo species. Moreover, because of the contribution of nitrogen (compared with oxygen in MoO₃ or H₃PMo₁₂O₄₀) in Mo₂N, the catalyst might be highly effective in the formation of active species. The studied catalyst could be easily reactivated by washing with acetonitrile and ethanol. Therefore, Mo₂N, especially supported on carbon (like Mo₂N@C), could be suggested as a promising catalyst in ODS.

Poster Presentation : **MAT.P-710**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Effect of substituents of corrole derivatives on generation of singlet oxygen

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The correlation between the molecular structures of three corrole derivatives (**PC**: 5,10,15-triphenyl corrole, **PFPC**: 5,10,15-tris(pentafluorophenyl) corrole, **MCPC**: 5,10,15-tris(p-methoxycarbonylphenyl)corrole) and their efficiencies for singlet oxygen generation was studied. Introducing electron-withdrawing fluorine atoms into the **PC** moiety led to a significant enhancement in singlet oxygen generation and facilitated intersystem crossing (ISC) due to enhanced spin-orbit coupling. Cyclic voltammetry experiments revealed a desirable linear relationship between the quenching rate constants and the oxidation potentials of the three corrole derivatives, indicating that the substituent effect is a critical factor governing the oxidation potential of photosensitizers for singlet oxygen generation.

Poster Presentation : **MAT.P-711**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Improving Lithium-Sulfur Battery Performances by Using N-containing Porous Aromatic Framework 41 as the Sulfur Support

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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%.

Poster Presentation : **MAT.P-712**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Conducting Polymers Built with Hydrogen-Bonding Biimidazole Scaffold as Anion-Responsive Chemical Fuse

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Conductivity-based chemical detection presents a number of advantages, including simple measurement setups and high sensitivity. Chemical fuse, in which specific stimuli shut down the electrical current, can be considered as a special case of detection in that the response itself is directly coupled to protective and preventive measures. Here, we disclose anion-selective structural disassembly of conducting polymers. This event occurs exclusively for strong hydrogen-bonding acceptor anions that engage in N-H \cdots X⁻ hydrogen bonding with the biimidazole units fused directly to the polymer backbone. When fabricated onto interdigitated microelectrodes, chemically triggered disassembly of the bulk material creates an open circuit. This presentation will discuss key design principles, synthetic implementations, and practical applications of designer polymers as an anion-responsive chemical fuse.

Poster Presentation : **MAT.P-713**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Removal of particulate matter in air by using zeolite-coated filters

Dong Kyu Yoo

Department of Chemistry, Kyungpook National University, Korea

Efficient removal of particulate matter (PM) in air is very important for a safe environment health, and conservation. In this study, we first applied zeolites, after coating onto substrates such as cotton and polyester, in PM removal from air and checked that aluminous zeolites could be very effective in the removal of PM. For example, NaX/cotton (NaX: ~20 wt% of cotton) showed 3.6- and 3.4-times the removal efficiency (RE) of pristine cotton for PM_{2.5} and PM₁₀ elimination, respectively, even though the pressure drop increased only slightly (by 9 Pa). In addition, NaX was much more effective than the widely applied metal-organic frameworks (MOFs) such as ZIF-8, UiO-66 and MOF-74 (or CPO-27), even though the porosity of NaX was much lower than those of the applied MOFs. Significantly, the quality factor (QF) and RE of the filters increased linearly with the increasing Al contents of the applied zeolites (with the same faujasite structure, namely NaY and NaX), suggesting the important role of Al and charge-compensating Na⁺ in PM elimination from air. Finally, it could be suggested that the PM removal is due to electrostatic interactions and aluminous zeolites (with charge-balancing cations) can be effectively used in the PM removal from air.

Poster Presentation : **MAT.P-714**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Microwave-assisted synthesis of reduced graphene oxide with hollow nanostructure for application to lithium ion battery

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

Reduced graphene oxide having a hollow nanostructure was synthesized using microwaves, and lithium storage characteristics were investigated. Graphite are widely used as LIB anode because they are stable and inexpensive, but have the disadvantage of low theoretical capacity (372mA h / g). Various nanostructures have been studied in LIB anodes to overcome the low capacity of graphite materials. Hollow spheres have an advantage in the anode electrode of LIB due to structural stability against volume change. In this study, reduced graphene oxide with hollow nanostructure was successfully synthesized using electrostatic interactions between building blocks and van der Waals forces. After 800th cycles at a current density of 1A / g, MRGO-HS maintained a capacity of 626mA h / g. In addition, when the charge/discharge rate capacity was measured stepwise in the current density range of 0.1-2 A / g, the discharge capacity of RGO rapidly decreased to 156 mA h / g even at the current density of 2 A / g, whereas MRGO-HS The electrode provided a capacity of 252 mA h / g. Even after 100th cycles have elapsed after the current density is restored at a charge/discharge rate of 0.1 A / g, the MRGO-HS capacity is 827 mA h / g, which is close to the original reversible capacity. Thus MRGO-HS provides higher capacity and better charge-discharge cycle stability than traditional synthesized reduced graphene oxide.

Poster Presentation : **MAT.P-715**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Particulate matters removal by using cotton coated with isomeric metal-organic frameworks (MOFs): Effect of voidage of MOFs on removal

Ho Chul Woo

Kyungpook National University, Korea

The presence of clean air is crucial to healthy life and sustainability; however, air pollution by various substances, especially particulate matters (PMs), is getting worse in recent decades. In this study, we explored three isomeric metal-organic frameworks (MOFs) such as MAF-5, MAF-6, and MAF-32 (MAF means metal-azolate framework, a sub-class of MOF), after coated on cotton, to remove PMs from the air. Isomeric MOFs were applied to identify an important parameter of MOFs in PM capture/removal since those MOFs have different characteristics (even have a close composition). It was observed that removal efficiency and quality factor (QF) of MAFs/cotton is linearly increased with increasing the voidage (v/v) of the investigated MAFs, suggesting the importance of the voidage of MOFs in PM capture. Moreover, we could explain how MAFs with small pore (compared with the size of PMs) is effective in interaction (for capture) between PM and MAFs. Finally, the MAF-6, the best MAF in PM removal among the studied MAFs, was much more efficient in PM removal than conventional or widely applied MOFs like ZIF-8 (for example, QF for PM_{2.5} of cotton, MAF-6/cotton and ZIF-8/cotton are 0.016, 0.060, and 0.030 Pa⁻¹, respectively).

Poster Presentation : **MAT.P-716**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Hybridization of Silver Nanoparticle with Layered Double Hydroxide for Efficient Surface-Enhanced Raman Spectroscopy

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Silver nanoparticle (AgNP) is an attractive material in terms of antibacterial, catalytic, electronic, and optical applications. Especially, AgNP takes advantage of surface-enhanced Raman spectroscopy (SERS) when they are prepared to have sharp edge and systematic orientation on a certain substrate. In this study, we suggested a synthetic method to obtain oriented AgNP on metal oxide by utilizing Ag-thiolate and layered double hydroxide (LDH) as precursor and template, respectively. First, nanosheets of Ag-thiolate and LDH was hybridized to have superlattice structure in layer-by-layer manner. Through reductive calcination process, the superlattice hybrid was transformed to metal oxide with AgNP array. Step-by-step characterization including powder X-ray diffraction, N₂ adsorption-desorption, electron microscopies, and X-ray photoelectron spectroscopy, revealed that the AgNP had good crystallinity and sufficient inter-particle gap for SERS performance at relatively high temperature (~ 600 °C). UV-vis diffuse reflectance spectroscopy showed that the calcination temperature affected both particle size and electronic structure of AgNP. Higher calcination temperature resulted in AgNPs with narrower band gap and higher plasmonic effect in the visible light region. To evaluate the SERS effect of prepared AgNPs, the 4-nitrothiophenol was utilized as target molecule. As a result, the AgNPs obtained at 600 °C presented the most effective SERS performance, exhibiting 50 times higher substrate enhancement factor than the one obtained at low temperature. We could suggest that hybrid of LDH and Ag-thiolate could be utilized as precursor for SERS material and that the calcination temperature is a determining parameter for SERS activity in current synthetic condition.

Poster Presentation : **MAT.P-717**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Local structure and magnetic properties change in layered double hydroxides upon chemical treatment

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¹*Energy and Material Engineering, Dongguk University, Korea*

The Mg-Fe and Ni-Fe layered double hydroxides (LDH) were treated with reductant, sodium borohydride and dilute nitric acid, respectively. The change in local structure before (p-MgFeLDH, p-NiFeLDH) and after treatment (r-MgFeLDH, r-NiFeLDH for reductant treatment and a-MgFeLDH, a-NiFeLDH for acid treatment) were investigated. According to X-ray diffraction pattern, it was confirmed that the crystalline phase and global crystallinity were well preserved after treatment. Electron microscopy exhibited that the particle size and shape of LDHs also did not significantly change upon treatment. However, X-ray absorption spectroscopy on Fe K-edge showed that the coordination number at first shell decreased in r-MgFeLDH and a-MgFeLDH compared with p-MgFeLDH implying the potential development of oxygen vacancy around Fe. On the other hand, the first shell of r-NiFeLDH and a-NiFeLDH preserved compared with p-NiFeLDH, indicating that NiFeLDH was resistant to chemical treatment in terms of vacancy evolution. Superconducting quantum interference device measurement showed that the paramagnetic property of LDH was generally preserved except reductant treated MgFeLDH. At 3 K, the M-H curve of p-MgFeLDH showed magnetic field dependent magnetization, implying paramagnetism. However, the M-H curve of r-MgFeLDH exhibited hysteresis with coercivity 182.5 Oe, suggesting the evolution of superparamagnetism. Spontaneous magnetization in r-MgFe-LDH would be attributed to the metallic disorder resulting from the oxygen vacancy.

Poster Presentation : **MAT.P-718**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Synthesis and magnetic field-driven assembly of core/shell silver-iron oxides nanowires

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Silver nanowires (Ag NWs) are one-dimensional anisotropic silver nanostructures with high electrical conductivity and low light extinction in the visible spectrum. Magneto-plasmonic nanoparticles (MagPlas NPs), especially magnetic composite nanostructures of gold and silver, are increasingly studied and developed as promising optical and sensing applications for the unique combination of plasmonic and magnetic properties. Therefore, in this study, the production and self-assembly of magnetoplasmonic core-shell Ag@Fe₃O₄ MagPlas NWs in the presence of external magnetic field are investigated. The Ag@Fe₃O₄ MagPlas NWs were synthesized using a two-step bottom-up solvothermal approach, in the presence of polyvinylpyrrolidone (PVP) as surface stabilizer. As a result, MagPlas NWs with overall aspect ratio of 74 were synthesized, with an evenly coated layer of magnetic-responsive of Fe₃O₄ nanoparticle clusters. The self-assembly of MagPlas NWs were induced by an external magnetic field, resulting in MagPlas NWs strictly aligned by the direction of magnetic field. The magnetic field strength, sample concentration and volume were found to be some of the factors affecting the quality of the assembled film. The interesting properties of MagPlas NWs as well as assembled NWs film hinting applications of this type of hybrid nanostructures in nanophotonic and optical devices.

Poster Presentation : **MAT.P-719**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Synthesis of ordered mesoporous Co₃O₄-based composite for CO preferential oxidation

Jung-ho Lee, Jae Ik Lee¹, Ji Man Kim*

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Preferential oxidation of carbon monoxide (CO-PROX) has got a great attention during decades, especially in proton exchange membrane fuel cell (PEMFC) field due to its simplicity and cost-effectiveness for the removal of CO in the H₂ fuel. This is because CO gas in the H₂ fuel contaminates Pt electrodes in PEMFC system, thus the performance of PEMFC diminished. Among various kinds of materials, noble metals were recognized as the promising candidates for effective CO-PROX reaction, however noble metal catalysts were not attractive due to their high costs. Transition metal oxides have been investigated for escaping from noble metal catalysis system. Co₃O₄ is a well-known CO-PROX catalyst which exhibits high catalytic performance (CO oxidation by O₂) at low temperature. In the preliminary research, ordered mesoporous Co₃O₄ showed high catalytic performances with T₅₀ of 68 °C due to its high surface area. In this work, we enhanced the CO-PROX performance of ordered mesoporous Co₃O₄ using 2 strategies: Co metal incorporation with ordered mesoporous Co₃O₄ framework and other transition metal doping. There were the studies of Co metal promotion in noble metal catalysts for improving CO-PROX activity. Also, other transition metal additives (Cu, Fe, etc.) in Co₃O₄ framework enhanced on the catalytic activity of ordered mesoporous Co₃O₄ due to the change of surface electronic structures. Thus, we prepared ordered mesoporous CoO, Co₃O₄, Co/Co₃O₄, and transition metal (Cu, Fe, etc.) and Co₃O₄ nanocomposites for CO-PROX by nano-casting method using KIT-6 silica hard template. The physicochemical properties of prepared catalysts were evaluated with XRD, BET, SEM&TEM with EDS, and TPR&TPD. The CO-PROX activity was improved when Co metal was incorporated with Co₃O₄ framework.

Poster Presentation : **MAT.P-720**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Plasmon-Driven Photocatalytic Intramolecular C-N Bond Formation Using Au Nanoparticles

Hyeonji Kim, Youngsoo Kim*

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Nitrogen-containing heterocyclic organic compounds have been a significantly important role in material science and pharmaceutical industries due to their good physical properties and excellent biological activities. In the last few years, Carbazole and its derivatives, one of the representative nitrogen-containing heterocyclic compounds, have been of great interest because of the application to drugs and optoelectronic materials. While many efforts to synthesize the Carbazole and its derivatives have been continued, the formation of the C-N bond under mild conditions has still remained an important task. However, a new strategy of which use of photocatalysts can be a key strategy to solve these problems. Among numerous types of photocatalysts, plasmonic photocatalysts can be one of the promising materials in terms of the use of visible light, which occupies about 50 % of the solar spectrum. In this study, we successfully synthesized Carbazole derivatives by inducing the intramolecular C-N bond formation of N-substituted aminobiphenyls using only Au nanoparticles and light. And, we also investigated the substituent effect of a functional group under mild reaction conditions.

Poster Presentation : **MAT.P-721**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Spontaneous Exfoliation of Two-Dimensional Molybdenum Oxide by Growth of Gold Nanoparticles

Jihoon Park, Youngsoo Kim*

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Since the discovery of graphene in the early 21st century, two-dimensional materials have been received much attention due to conductivity, optical properties, and mechanical strength that differ from bulk materials. Two-dimensional material is a substance with a thickness of a few nanometers and the vertical thickness is settled by multiple single layers, which interact with van der Waals force. In theory, the physical properties of two-dimensional materials become much stronger, when the thickness is reduced to a single or few-layer. Even though many kinds of the method to make reduced thickness have been proposed, earlier methods have trouble in control the thickness that affects the properties of the two-dimensional material. In this study, we proposed a new way to make single or few-layer MoO₃ nanosheets by the growth of gold nanoparticles inside layers. We firstly investigated the optimal condition of intercalation like the composition of solvents, temperature, time, and etc. Then, we conducted an experiment for the growth of gold nanoparticles. The exfoliated MoO₃@Au heterostructures were characterized by UV-Vis spectrophotometer, XRD, and TEM. As a consequence, the MoO₃ nanosheets with immobilized gold nanoparticles were observed and the reduced thickness of MoO₃ clearly was found.

Poster Presentation : **MAT.P-722**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Aggregation-induced phosphorescence enhancement effect of iridium(III) complexes for deep-red to near-infrared emissive and solution-processable OLEDs

Taehyun Kim, Dasol Chung, Taiho Park*

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Low bandgap luminophores have troublesome due to the vulnerability of tiny emissive band gap towards counteractive triplet-triplet annihilation(TTA) and non-radiative decay by vibrational energies. Therefore, to avoid concentration quenching and enhance emissive properties, we synthesized aggregation-induced emissive phosphorescent iridium(III) complexes with introducing several substituents such as electron withdrawing -phenyl(Ir2), -ethyl ester(Ir3) and -trifluoromethyl(Ir4) groups on the N-coordinating quinolone moiety of a (benzo[b]thiophen-2-yl)quinoline cyclometalated ligand along with ancillary picolinate. Moreover, we investigated the origin of aggregation-induced emission effect and its electronic characteristics of excited states by comparing with unsubstituted iridium complex(Ir1). Based on density functional theory(DFT) calculation and single crystal X-ray diffraction(XRD) analysis, the molecules were deeply analyzed. Eventually, we fabricated organic light emitting diodes by solution-process using aggregation induced emissive Ir2 complex which is exhibited maximum external quantum efficiency of 7.29%.

Poster Presentation : **MAT.P-723**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Effect of Mo doping for improved electrochromic properties of WO₃ thin films

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Doping with transition metal oxides is a very efficient way to modify the structural, optical and electronic properties of the WO₃ which could influence its electrochromic properties. In this study, we synthesized pure and Mo-doped WO₃ nanoparticles by co-precipitation method and characterized by XRD, FE-SEM, EDS and UV-Visible spectrometer. Thin films of pure and Mo doped WO₃ were coated on indium tin oxide(ITO)/PET substrates by wet coating technique. The electrochemical and electrochromic performance of the films were measured by cyclic voltammetry in 0.1M LiClO₄ electrolyte solution. Compared to the pure WO₃, Mo-doped WO₃ films show improved electrochromic properties with fast coloring speed(16.9s), large optical modulation (61.6% at 550 nm), high charge density (36.6mC/cm²) and excellent durability.

Poster Presentation : **MAT.P-724**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Diamond-like Semiconductors for All-solid-state Batteries

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The all-solid-state battery is a battery composed by the solid electrolyte of the lithium-ion battery. Liquid electrolytes have thermal stability problems such as explosions, however, all-solid-state batteries have the advantage of having a higher structural safety than conventional lithium-ion batteries, reducing the risk of impact and damage. Therefore, all-solid-state batteries are promising as next-generation lithium-ion secondary batteries. In this work, we synthesized the diamond like structures (DLSs) compound, Li_2MGeS_4 and $\text{Li}_4\text{MGe}_2\text{S}_7$. DLSs are capable of various variations such as binary to quaternary as cations are arranged at Zn site of zinc blend structure. Depending on the transition metal element located at the cation site, DLSs has ccp and hcp anion framework according to the element packing. $\text{Li}_4\text{MGe}_2\text{S}_7$ has more lithium content than Li_2MGeS_4 and the tetrahedral of Li site of $\text{Li}_4\text{MGe}_2\text{S}_7$ coordinated by S anion is slightly distorted, in these reasons, the Li ion conductivity of $\text{Li}_4\text{MGe}_2\text{S}_7$ is expected to be higher than Li_2MGeS_4 . The compounds are synthesized by solid-state reaction and analyzed using PXRD and Rietveld refinement. Li ion conductivity is measured by electrochemistry impedance spectroscopy.

Poster Presentation : **MAT.P-725**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Application of Au Nanoparticles to Various Intermolecular Coupling Reaction

Juhee Ha, Youngsoo Kim*

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The intermolecular coupling is one of the important synthetic strategies for forming a new bonds in organic chemistry, medicinal chemistry, and biochemistry. Organic chemists have been developed many types of intermolecular coupling reactions so far. Conventionally, most coupling reactions have used transition metal-based catalysts such as Pd, Ni, and Cu, and these reactions have required high reaction temperatures and toxic chemicals to obtain new materials. To overcome crucial issues such as harsh reaction conditions and environmental problems, various alternative synthesis strategies have been proposed. Among those various ways proposed, the photocatalysis technique which uses catalysts and light could be a rational approach due to need mild reaction condition and the use of less toxic chemicals. Recently, various research groups have conducted much researches with gold nanoparticle photocatalyst to drive a chemical reaction. In this study, we have introduced various carbon-carbon coupling reaction like a Suzuki, Sonogashira, Stille, and Ullmann cross-coupling using plasmonic Au nanoparticles and visible light. Consequently, we confirmed that new organic molecules were successfully coupled from various type of reactions, as well as the results implies that plasmonic gold nanoparticles can be applied as a versatile catalyst for organic synthesis.

Poster Presentation : **MAT.P-726**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Broadband-assisted upconversion photoluminescence with organic sensitizer

Seung Ju You, Doo-Hyun Ko*

Department of Applied Chemistry, Kyung Hee University, Korea

Lanthanide-doped upconversion nanoparticles (UCNPs) have received considerable attention due to their unique optical characteristics that convert light from the near-infrared to the ultraviolet or visible region. However, extremely poor absorption profiles, such as low absorption coefficient and narrow band absorption, distracted the application of UCNPs. This study proposed a novel strategy to fabricate the solid-phase upconversion film, overcoming the restricted optical properties of UCNPs by incorporating additional organic sensitizer. A significantly high and broad absorption coefficient of organic sensitizer facilitated upconversion excitation. The organic dye assisted upconversion photoluminescence intensity was remarkably amplified as a three-order degree compared to that of pristine UCNPs. As a proof of concept, the energy transfer and re-absorption behaviors from dye to UCNPs were characterized through time-resolved optical measurement. Hence, beyond the intrinsic limitations of UCNPs, our approach suggested versatile applications for optical memory, photonic transistor, and photovoltaic system.

Poster Presentation : **MAT.P-727**

Material Chemistry

Zoom 18 FRI 15:00~16:00

Multi-functional wave-converting platform via scattering enhanced

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Kyung Hee University, Korea

¹*Department of Applied Chemistry, Kyung Hee University, Korea*

Quantum dot have recently been considered the key factor for the light-emitting materials in the future display due to their inherent optical characteristics; color-tunability, high photoluminescence quantum yields, and absorption coefficient. We developed the assembly of silica microsphere and quantum dot (SQD) to improve the optical performance of quantum dot (QD) nanoparticles, ameliorating the intrinsic properties of QD nanoparticles. The meticulous optical behaviors and finite-difference time-domain calculation were simultaneously carried out to demonstrate the size-dependent scattering characteristics. The SQD-incorporated film was fabricated to achieve attachability, transparency, and flexibility. This strategy exhibited the expanded light path and absorbance at the excitation region via the SQD-driven scattering phenomena. The photoluminescence of the suggested film was significantly amplified up to a 3-folded increase, which maintained the high transparency and outstanding durability. We further fabricated the SQD-incorporated macroscale film to validate the physical properties and applicability. Consequently, our approach could sufficiently promote versatile applications for the future quantum-based display industry.

Poster Presentation : **MAT.P-728**

Material Chemistry

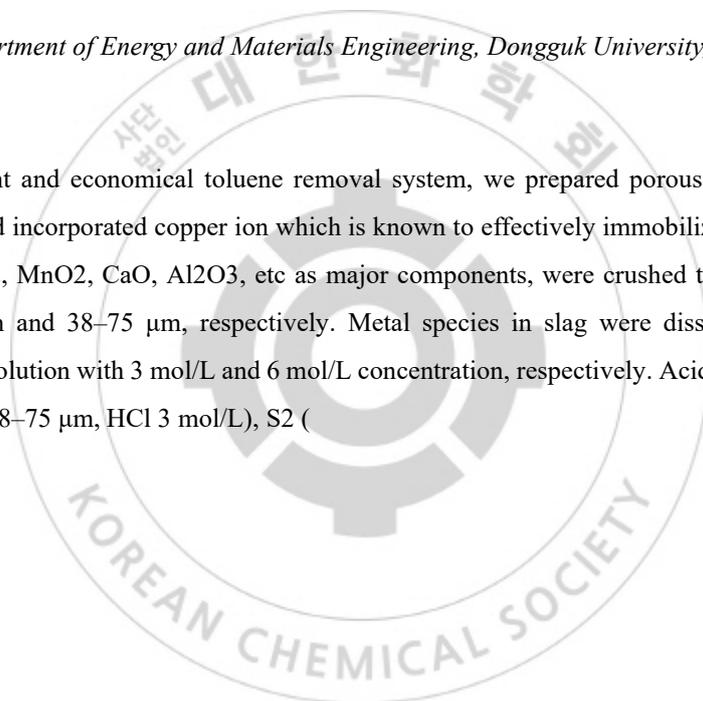
Zoom 18 FRI 15:00~16:00

Synthesis of copper-incorporated porous silica from industrial waste for effective removal of gaseous toluene

Jio Kim, Do-Gak Jeung, Namho Kim, Jae-Min Oh*

Department of Energy and Materials Engineering, Dongguk University, Korea

To prepare efficient and economical toluene removal system, we prepared porous silica network from industrial waste and incorporated copper ion which is known to effectively immobilize toluene. First, slag lumps having SiO₂, MnO₂, CaO, Al₂O₃, etc as major components, were crushed to small particles and sieved to < 38 μm and 38–75 μm, respectively. Metal species in slag were dissolved by treating in hydrochloric acid solution with 3 mol/L and 6 mol/L concentration, respectively. Acid treated sample were designated as S1 (38–75 μm, HCl 3 mol/L), S2 (



Poster Presentation : **MAT.P-729**

Material Chemistry

Zoom 18 FRI 15:00~16:00

A Stacking-based ensemble learning for prediction of impact strength for polymer composite materials

Inhyeok Song, Dong Ryeol Shin, Sung Kwang Lee*

Department of Chemistry, Hannam University, Korea

In order to produce polymer composite material for industrial use, it must satisfy the physicochemical properties suitable for use. Having the suitable physicochemical properties is time consuming and expensive because the conditions such as the materials, its composition and process are optimized. In this study, we developed predictive models based on the impact strength data of polymer composite materials. Optimized models that can predict impact strength through a combination of variable using material properties, its composition, process variables and individual properties of polymers, fillers, and additives. Several tree-based composite models (RF, GBT, EXT, XGBoost, LightGBM) were used as model algorithms, and the performance of the stacking algorithm combining the results of each model was also compared. The hyperparameter and feature selection of all models were optimized with the RMSE of the internal bootstrapping validation, and the predictability of each models was evaluated through the performance of the external validation set. The developed model will be an alternative to reduce the time and cost of developing composite materials with desired mechanical properties.

Poster Presentation : **MAT.P-730**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Enhancement of electromagnetic wave absorption using oxygen deficient ferroelectric particles-based composite

Baek Kyungnae, Jerome Hyun^{1,*}

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Perfect microwave absorption is becoming essential for preventing electronic malfunction in electronic devices and control systems such as wireless vehicles. In order to improve the absorption, impedance ($\eta = \sqrt{\mu/\epsilon}$) should be matched between film and surrounding to prevent power loss from reflection. Furthermore, miniaturization of electronic components demands the need for thinner of microwave absorption film. To become thinner, the film should possess a high refractive index ($n = \sqrt{\epsilon\mu}$). To this end, magnetodielectric composite with high refractive index and good impedance matching are widely employed. In this study, we explored the microwave absorption properties of oxygen deficient BaTiO₃ particles prepared by the Molten Salt synthesis (MSS) method. This result suggests that the oxygen vacancies led to improve the dielectric constant of ferroelectric BaTiO₃ particles.¹ Additionally, we mixed this oxygen deficient BaTiO₃ particles with soft magnetic FeSiAl flakes by heat pressing.² This magnetodielectric composite exhibits significantly improved magnetic permeability and dielectric permittivity, which result in high refractive index for thinner film. This result indicates the BaTiO₃ particles spatially separate the FeSiAl flakes, which suppresses eddy currents, and induces strain in the flakes, which improves the saturation magnetization, resulting in enhanced permeability. Also, this composite shows that perfect absorption (60dB) is achieved at a unique thickness that is an order of magnitude less than a quarter wavelength. (1) Baek, K.; Lee, S.-Y.; Doh, S.-G.; Kim, M.; Hyun, J. K. J. Mater. Chem. C 2018, 6, 9749-9755. (2) Baek, K.; Doh, S.-G.; Jeong, W.; Lee, O.; Hyun, J. K. J. Alloys Compd. 2021, 159075.

Poster Presentation : **MAT.P-731**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Morphology Control for High-Performance Organic Photovoltaics via Solvent Additives

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Department of Applied Chemistry, Kyung Hee University, Korea

High-performance organic photovoltaics (OPVs) exhibit nanoscale phase-separation in bulk-heterojunction (BHJ) layer irrespective of the spectra compatibility. As one of the representative methods, insertion of solvent additives facilitates phase interpenetrating networks within donors and acceptors, generating free charge carriers and building charge transport pathways. In this study, we propose the primary approach to morphology control via solvent additives. We scrutinize the morphological variation depending on two types of solvent additives thereof, which activate or inhibit the aggregation of polymer donors. The photovoltaic characteristics are definitely manipulated according to the quantity and type of each additive. In particular, under AM 1.5G and LED irradiation, we acquire power conversion efficiencies of 13.56 and 23.49%, which are derived from the improved fill factors of 71.25 and 72.24%. Hence, our approach can adequately provide the facile methodology for modulating the photovoltaic parameters.

Poster Presentation : **MAT.P-732**

Material Chemistry

Zoom 18 FRI 16:00~17:00

In Situ Synthesis of Trimeric Ruthenium Cluster-Encapsulated ZIF-11 and Its Carbon Derivatives for Simultaneous Conversion of Glycerol and CO₂

Kyung-Ryul Oh, Young-Uk Kwon^{*}, Young Kyu Hwang^{1,*}

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¹*Carbon Resources Institute, Korea Research Institute of Chemical Technology, Korea*

Stable, high-performance noble-metal catalysts have proven effective for obtaining lactate (LA) and formate (FA) from simultaneous conversion of glycerol and carbonate as a CO₂ source. For this purpose, we developed a novel method reported herein for the synthesis of Ru nanoparticles (NPs) supported on graphitic nanoporous carbon (Ru/NCT, T = pyrolysis temperature). The Ru/NCT catalysts were prepared by in situ encapsulation of trimeric ruthenium clusters in ZIF-11 pores, with a subsequent pyrolysis process. The pyrolysis temperature affected the size and crystallinity of Ru NPs and the textural properties of the ZIF-11-derived carbon. Optimization of reaction parameters such as CO₂ source, reaction temperature, reaction time, and glycerol/carbonate ratio resulted in Ru/NCTs with significantly higher turnover number (TON) and space-time yield (STY) of the desired products (LA and FA). Moreover, these Ru/NCTs were stable even after three consecutive recycle tests without leaching of active metal or notable structural change. The correlation of reaction performance and detailed characterization revealed that large Ru NPs with high crystallinity exhibit superior catalytic activity for the combined dehydrogenation-hydrogenation reactions that yield the desired products.

Poster Presentation : **MAT.P-733**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Fusion Complex of Silver Nanoparticle-Porous Silicon Microparticle as a Contrast Agents in Computed Tomography Scan

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With the rapid development of diagnostic imaging techniques, diagnosing of diseases at the early stage has become possible, extending the lifespan and improving the quality of life. In particular, the invention of contrast agents increases diagnosis accuracy by enhancing image quality. Therefore, finding contrast agents with high contrast intensity and low immune response turns out to be a big interest in the medical field. We developed a fusion complex of silver nanoparticles (AgNPs) and porous silicon microparticles (pSiMPs) as an image-guided localization agent for the computed tomography (CT) scanning of the lungs. We verified the grafting of AgNPs and oxidized pSiMPs through various analytical equipment, including a scanning electron microscope, Fourier transform infrared spectroscopy, X-ray diffraction, and energy-dispersive X-ray spectroscopy. To confirm its applicability in the mammalian system (animal model), we injected the compound into the lungs of rabbits and rats. As a result, rabbit and rat lung CT showed strong aggregation signals for up to 1 hour without spreading at the injection site. In addition, it showed negligible toxicity and immune response. Hence, we suggest this fusion complex as a new image-guided localization agent of CT scans for lung cancer surgery. Ref: ACS Biomaterials Science & Engineering, 2020, 6, 8, 4390-4396.

Poster Presentation : **MAT.P-734**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Synthesis of the Web-above-a-Ring (WAR) and their Single-Particle Surface-Enhanced Raman Scattering

Soohyun Lee, Sungwoo Lee, Sungho Park*

Department of Chemistry, Sungkyunkwan University, Korea

Surface-enhanced Raman Scattering (SERS) is an important, highly sensitive technique for chemical and biological analysis, which critically depends on the morphology of metal structures. Great efforts have been made to fabricate metallic nanostructures with nanoscale gap. Nanoscale gaps between adjacent plasmonic nanostructures exhibit large enhancement of electromagnetic field, which are often termed as electromagnetic hotspots. Recently, several synthetic methods have been used to synthesizing metal nanoparticles. Among them, galvanic replacement reaction is widely used method for the fabrication of hollow nanostructures. Galvanic replacement reaction provides a simple but versatile way of converting less noble metallic solid nanoparticles into structurally complex hollow nanostructures composed of more noble metals such as Au, Pt, and Pd. Herein, we report complex nanostructures utilizing Pt-Au nanoring as a core, a subsequent concentric growth of Ag around the core nanoring, and the galvanic replacement reaction between Ag and Au ions for synthesizing Pt-Au nanoring-AuAg porous nanoweb. These web-above-a-ring (WAR) particles are SERS active in single particle scale, due to the plasmonic coupling between the core Pt-Au nanoring and AuAg porous shell. By controlling the thickness of Ag layer, we can precisely control the intra-gap distance between Pt-Au nanoring and Au porous core-shell from 4 nm to 8 nm. Homogeneous synthesis of WAR nanoparticles with single particle SERS activity enables us to utilize them for a SERS substrate.

Poster Presentation : **MAT.P-735**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Development of self-assembled protein structure using Transferrin with Fe³⁺ ion for cancer therapy capable of drug release by pH control

Tomoyuki Tachibana, Akihiro Yabuki, Ji Ha Lee*

Graduate School of Advanced Science and Engineering, Hiroshima University, Japan

Two kinds of drug carriers with Transferrin, which were HOLO (with Fe³⁺ ion) and APO (without Fe³⁺ ion) were developed by self-assembly. The self-assembled drug carriers showed different aggregation behaviors. In the case of HOLO Transferrin, nanoparticles were formed. On the other hand, hydrogels were formed in salt solvent conditions. We characterized self-assembled drug carriers by UV-vis spectra and dynamic light scattering (DLS) and flow field fractionation (FFF) to determine the loading ratio, size. The morphology of drug carriers was observed by SEM. In the event of hydrogel, we controlled the drug release at different pH conditions and temperatures in detail. Additionally, the cytotoxicity of drug-loaded Transferrin was evaluated. We proposed the potential clinical medications based on the protein assembly, particularly for overcoming problems with solubility in aqueous systems for drug delivery systems for cancer therapy.

Poster Presentation : **MAT.P-736**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Scale-up synthesis of high fluorescent FeSe quantum dot in aqueous condition

Youngeun Choi, Yujin Choi¹, Jaebeom Lee^{1,*}

Chemical Engineering and Applied Chemistry, Chungnam National University, Korea

¹*Chemistry, Chungnam National University, Korea*

Iron chalcogenides hold considerable promise for energy conversion and biomedical applications. These iron-containing quantum dots also serve as a safe alternative to the conventionally used metal-chalcogenide systems in which the heavy metal component is usually toxic. Here, a successful synthesis of Iron selenide(FeSe) quantum dots(QDs) is reported in an aqueous system using glutathione(GSH) and L-cysteine(Cys) as surfactants. Reaction was optimized by controlling reaction pH, time and temperature to improve the quantum yield. Then, the QDs with highest QY were characterized by transmission electron microscopy (TEM) and optical spectrophotometry. Scale-up synthesis was carried out where 100~1000-mL reactors were used to synthesize QD up to 0.1g per batch. Furthermore, the prepared FeSe NPs exhibited intense light blue fluorescence on ultraviolet light exposure, which also displays strong photoluminescence and relatively high quantum yield in an aqueous system.(c.a.20%) This novel strategy, based on the synthesis of Iron chalcogenides quantum dots in an aqueous system, has the potential to increase significantly towards in-vivo bio-imaging and sensing.

Poster Presentation : **MAT.P-737**

Material Chemistry

Zoom 18 FRI 16:00~17:00

DNA activated-MWCNT@paper sensor for the simple and fast detection of microcystin-LR

Myeongsoon Lee, Jeong Eun Kim¹, JiHyeon Mun¹, Don Kim^{*}

Department of Chemistry, Pukyong National University, Korea

¹*Department of chemistry, Pukyong National University, Korea*

An environmental sensor for microcystin-LR(MC-LR) detection was prepared from bioactivated multiwall carbon nanotubes (MWCNTs), which were activated by immobilization of a specially designed deoxyribonucleic acids (DNA: MC-LR targeted aptamer), deposited micro-pore filter paper. The sensor could assay MC-LR level in freshwater within the world health organization guideline (≤ 1.0 ng/mL) with the detection limit of 0.15 ng/mL by the measurement of the electrical resistance change with spring-loaded probe contact within 1 h. The selective interaction between MC-LR and the aptamer would be the main detection mechanism.

Poster Presentation : **MAT.P-738**

Material Chemistry

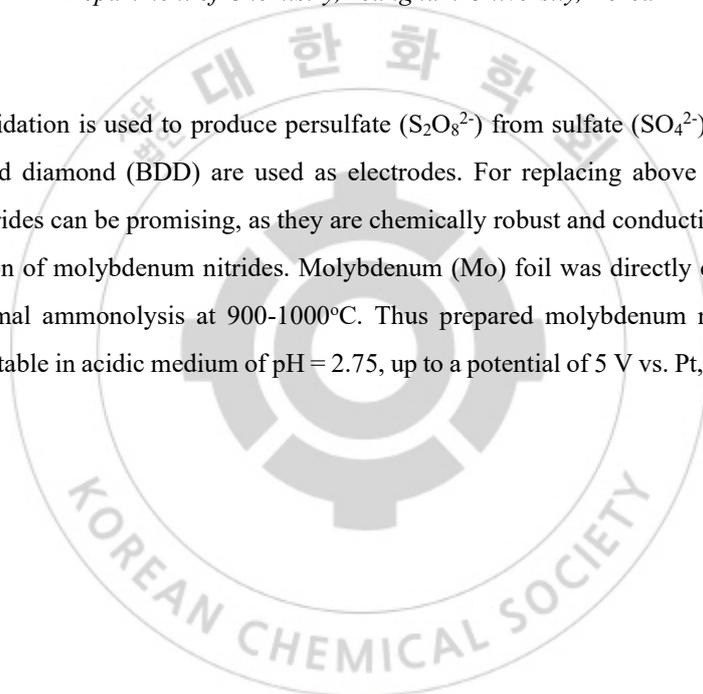
Zoom 18 FRI 16:00~17:00

Molybdenum nitride anode for electrooxidation of sulfate to persulfate

Dong Hyun Lim, Young-il Kim*

Department of Chemistry, Yeungnam University, Korea

The electrolytic oxidation is used to produce persulfate ($S_2O_8^{2-}$) from sulfate (SO_4^{2-}), for which platinum (Pt) or boron-doped diamond (BDD) are used as electrodes. For replacing above expensive materials, transition metal nitrides can be promising, as they are chemically robust and conductive. In this regard, we explored preparation of molybdenum nitrides. Molybdenum (Mo) foil was directly converted to MoN or Mo_2N by the thermal ammonolysis at 900-1000°C. Thus prepared molybdenum nitride electrode was electrochemically stable in acidic medium of pH = 2.75, up to a potential of 5 V vs. Pt, and a current density of 0.2 A/cm².



Poster Presentation : **MAT.P-739**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Plasmonic nanosphere oligomers binding to metal linker using synthetic chemical toolkit

Jeongwon Kim, Sungho Park*

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In nanoscience, self-assembly of nanoparticles is a powerful tool that can control material property, especially in plasmonics, sensing, surface-enhanced Raman scattering (SERS) and optics. Despite many approaches in self-assembly, there still remain challenges in obtaining high yields, additional steps in preparation, filtering, stability and accessibility to chemical and biological analyte. Meanwhile, recent research has focused on the study of complex nanoframes, which can be regarded as the assembly of nanospheres, nanorods and nanorings. Herein, we designed the nano oligomers (dimer, trimer and hexamer) linked with metal bridges. Such complex shapes can be realized by multistep synthetic steps. The synthetic pathways undergo as follows. (I) Sphere selective growth on the vertex region through Echem control : Shapes of Au nanoparticles (nanorod, nanoprism and nano-hexagon) are precisely controlled by simultaneous reaction of Au growth on tips and edge etching. (II) Selective Pt protection on the Au nanosphere domain: Pt⁴⁺ ions are selectively reduced at the sphere region of the Au nanoparticles. (III) Body-selective Au etching and sphere-selective protection of Au nanosphere domain: original Au domain is exclusively etched to Au⁺ ions, whereas sphere regions are preserved by Pt protection. (IV) Sphere-selective Au growth on the nano oligomers: Au⁺ ions are selectively reduced to certain sites of the AuPt nanospheres. Furthermore, plasmonic properties of the nano oligomers reveal that these nanostructures exhibit combination of nanospheres and nanobridges. This on-demand colloidal synthesis of complex nanostructure will pave the new way for exploiting new generation of nanoparticles such as linker-free assembly of nanoparticles.

Poster Presentation : **MAT.P-740**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Synthesis of Nanoporous Structure Embedded Au Nanorings for Single-Particle SERS Measurement

Sungwoo Lee, Sungho Park*

Department of Chemistry, Sungkyunkwan University, Korea

We suggest a strategy of synthesizing Pt@Au nanorings with near-field focusing capability at the center where single-particle surface-enhanced Raman scattering (SERS) could be readily observed. We utilized Pt@Au nanorings for light-absorber, and the absorbed light could be focused at the center with the support of Au nanoporous structure. We synthesized nanoporous structure embedded Au nanoring structure (Au nanolens) which has both Pt@Au nanoring and Au nanoporous structure via Galvanic replacement between Au ions and Ag block at the inner domain of the Pt@Au nanorings. In this step, we selectively deposited Ag at the inner domain of the Pt@Au nanorings through electrochemical potential-tuned growth control and different surface energies of inner and outer domain of nanoring. Then, the central nanoporous structure was synthesized through the Galvanic exchange reaction of sacrificial Ag block with Au ions leading to the Au nanoring with Au nanoporous structure at the center. We monitored the synthetic procedure by monitoring their localized surface plasmon resonance (LSPR) profiles using UV-vis-NIR-spectrophotometer. When we controlled the rim thickness of the Pt@Au nanorings, the inner diameter of the Au nanolens was accordingly tuned to maximize near-field focusing ability, which enabled us to obtain the reproducible and light-polarization independent measurements of single-particle SERS. Through the theoretical simulation, the near-field electromagnetic field focusing capability was confirmed through single-particle SERS measurement.

Poster Presentation : **MAT.P-741**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Electrochemical and Photoelectrochemical Oxygen Evolution Reactions by Group X Hetero-Metal Oxides

Junhyeok Seo^{*}, Dongwan Yoo

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To build a renewable energy system, electrochemical and photoelectrochemical water splitting methods must be improved. In this research, we synthesized Group X hetero-metal oxides and investigated the (photo)electrochemical properties for the potential application to oxygen evolution reaction (OER). The Group X hetero-metal oxides nanoparticles as deposited on a nanorod-shaped TiO₂ surface exhibited fascinating chemical and photoelectrochemical properties. The hetero-metal oxides increased OER activity in a systematic order by suppressing the charge recombination on the TiO₂ surface, as well as modulating the TiO₂ band gap. The OER activity increased as follows: PtO << Ni/NiO < PdO+Ni/NiO < PtO_x+Ni/NiO. Notably, the Pt/PtO_x+Ni/NiO hetero-metal oxides acted as the most efficient cocatalyst on the TiO₂ surface with the photocurrent of 2.62 mA/cm₂ at 1.23 V vs. RHE and 70 % IPCE value, which is ~4 times higher than that of a pristine TiO₂.

Poster Presentation : **MAT.P-742**

Material Chemistry

Zoom 18 FRI 16:00~17:00

A hybrid complex of dipolar fluorophore and serum albumin: Visualization of mitochondria and mouse intestine

Jongmin An, Dokyoung Kim^{1,*}

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¹*College of Medicine, Kyung Hee University, Korea*

A rationale of the fluorophore-protein hybrid complex has been spotlighted to improve the ability of fluorophore and to visualize various substrates, including biomolecules and cellular organelle. Among them, the tracing of a particular site in the organism is drawing attention to the field of disease diagnosis, translation medicine, and basic science. Herein, we disclosed a small molecule that is based on naphthalene backbone with donor-acceptor type and hybrid complex with the molecule and serum albumin (SA) for the first time. The naphthalene-based small molecule, IPNHC, was synthesized through a cascade reaction under the condition of the Mitsunobu reaction using diisopropyl azodicarboxylate (DIAD) and triphenylphosphine (PPH₃). Its photophysical properties with SA were systematically identified, and the IPNHC-SA hybrid complex demonstrated high quantum yield, the stability of fluorescence, and specificity for mitochondria and intestine under the UV irradiation as well as two-photon (TP) tissue imaging with negligible background after tail vein injection into a mouse. The present finding holds promise for applications of the hybrid complex of fluorophore-protein to a relatively simple and straightforward following of mitochondria- and intestine-related diseases at clinical sites. [Ref: 1]References[1] J. An et al., J. Mater. Chem. B, 2020, 8, 7642-7651

Poster Presentation : **MAT.P-743**

Material Chemistry

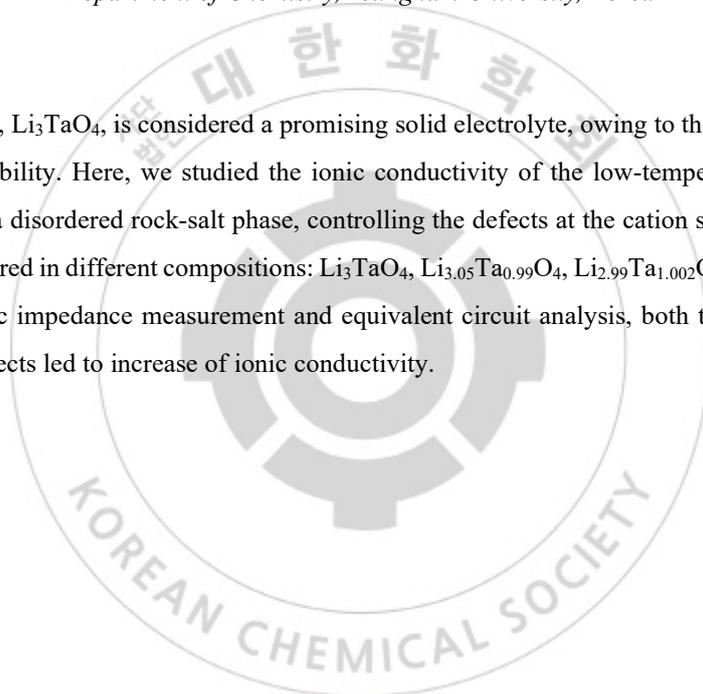
Zoom 18 FRI 16:00~17:00

Defect control and ionic conductivity of disordered rock-salt Li_3TaO_4

Chaeun Kim, Young-il Kim*

Department of Chemistry, Yeungnam University, Korea

Trilithium tantalate, Li_3TaO_4 , is considered a promising solid electrolyte, owing to the high Li content and electrochemical stability. Here, we studied the ionic conductivity of the low-temperature polymorph of Li_3TaO_4 , which is a disordered rock-salt phase, controlling the defects at the cation site. Particularly, four samples were prepared in different compositions: Li_3TaO_4 , $\text{Li}_{3.05}\text{Ta}_{0.99}\text{O}_4$, $\text{Li}_{2.99}\text{Ta}_{1.002}\text{O}_4$, and $\text{Li}_{2.98}\text{Ta}_{1.004}\text{O}_4$. According to the ac impedance measurement and equivalent circuit analysis, both the vacancy-type and interstitial-type defects led to increase of ionic conductivity.



Poster Presentation : MAT.P-744

Material Chemistry

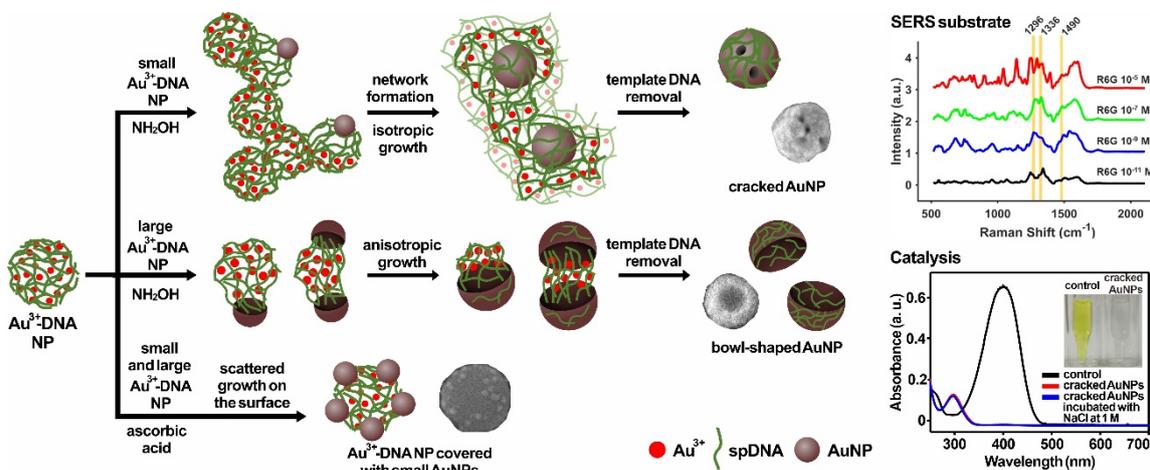
Zoom 18 FRI 16:00~17:00

Spherically Condensed Au³⁺-DNA Nanoparticles and Their Controlled Sacrificial Reduction into Functional Gold Nanoparticles

Won Kyu Lee, Jae-Seung Lee*

Department of Materials Science and Engineering, Korea University, Korea

Despite significant advances in understanding reversible condensation properties of DNA with metal ions (Mn⁺s), the synthesis of spherically condensed Mn⁺-DNA nanocomposites and their reduction have been rarely investigated. We synthesized a positively charged Au³⁺ complex via ligand-exchange, which induces spherically condensed DNA nanoparticles (Au³⁺-DNA NPs) through coordination and electrostatic interaction. We selectively reduced Au³⁺-DNA NPs into functional Au nanostructures with excellent catalytic activities and SERS properties using different types of reductants. We also presented how the Au³⁺-DNA NPs play a role as dynamic templates during their reduction for the synthesis of Au nanostructures with unique morphologies (cracked NPs, bowl-shaped NPs, and small NPs). We found that the growth mechanism of the Au³⁺-DNA NPs is completely different from the conventional nucleation-growth process and is dependent on their multistep shape-transition. Based on our approach, other soft materials such as proteins and RNA can be employed as dynamic templates with different metal ions for the synthesis of various metal nanostructures.



Poster Presentation : **MAT.P-745**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Novel Design of Pyridothiadiazole based Non-fused Ring Acceptors for Organic Solar Cells

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Developing bulk-heterojunction (BHJ) organic solar cells (OSCs) have attracted the interest of researchers over recent past years due to their cost-effective and ease of processing, advantages of transparency, lighter weight, device engineering and prospect in producing large-scale OPV modules. However, the most of the features of NFAs includes a tedious multistep synthesis to afford a large fused-ring backbone structure, that limits their applicability to commercial applications. In this work, we report a series of nonfused-rings NFAs, WHC-1, WHC-2 and WHC-3, based on an A-D-A'-D-A design architecture, containing an electron-deficient pyridothiadiazole central unit and tuned their energy bandgap by tailoring and orienting the nitrogen of the pyridothiadiazole unit. Tailoring the structure by increasing the backbone chain and orienting the central core lead to fine tuning of the energy levels, optical properties and molecular crystallinities. Moreover, a decent power conversion efficiency is achievable by WHC-1 by blending along with an appropriate donor material. The higher chain length of the A-D-A'-D-A units in the NFAs (WHC-2 and WHC-3) resulted a narrow band gap acceptors with equal chain lengths but different orientation of the A' unit. In the present work, we will demonstrate the potential of A-D-A'-D-A type nonfused NFAs and their corresponding narrow band gap NFAs for high-performance OSCs. Further development of non-fused ring acceptors (NFRAs) by employing appropriate and suitable D-A π -conjugated building units and optimizing the side-chain to fabricate solar cell of narrow band gap NFAs for high efficiency organic solar cell

Poster Presentation : **MAT.P-746**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Simple and Rapid Synthesis of Highly Efficient Cesium Lead Halide Perovskite Nanocrystals by Ultrasonication Method

Sang Yoon Lee, Geonho Lee¹, Seong Hyun Jang¹, Jun Choi^{1,*}

*Human Convergence Technology R&D Department, Korea Institute of Industrial Technology(KITECH),
Korea*

¹*Human Convergence Technology R&D Department, Korea Institute of Industrial Technology, Korea*

Cesium lead halide perovskite nanocrystal has high potential as a next-generation display light emitting material with bright, low-cost, tunable emission wavelength, high photoluminescence quantum yield, and narrow full width at half maximum. Therefore, it is being synthesized in various methods. Conventional methods such as hot injection method and ligand-assisted re-precipitation technology are difficult to manufacture on a large scale due to complex conditions and long synthesis time. In this study, we introduce an optimized ultrasonication method that improves the stability of CsPbX₃ perovskite nanocrystals and is suitable for rapid and mass-producible synthesis. The suggested ultrasonication method was quick and simple to synthesize in minutes by putting all the precursors in one-pot. As a result, it was possible to obtain a large scale of perovskite nanocrystals compared to other methods, and showed stable and high optical efficiency. Through these processes, we confirmed the excellent photophysical properties of the fabricated perovskite nanocrystal inks, the photoluminescence and electroluminescence.

Poster Presentation : **MAT.P-747**

Material Chemistry

Zoom 18 FRI 16:00~17:00

The Synthesis and Characterization of Highly Water Soluble Dimeric Triphenylmethane Acid Dyes and Its Application for the Digital Textile Printing

Seong Hyun Jang, Geonho Lee, Sang Yoon Lee¹, Jun Choi^{*}

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Digital Textile Printing (DTP) is a process of printing ink with micronized dots using an inkjet printing machine to realize a designed pattern or image directly on a fabric. Digital textile printing has many advantages as follows. Firstly, it shortens the whole process time due to the elimination of screen plate manufacturing process. Secondly, it is an eco-friendly process that can reduce the environmental pollution such as waste-water. Finally, this printing method is suitable for small quantity batch production that can meet the needs of various consumers in a short time. Since the 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 novel 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 theory using G16 package b3lyp 6-31g (d) level, geometrical information between the moieties constituting the dyes 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. In addition, the ink formulation recipe was optimized using prepared dyes for high speed DTP, the prepared inks formed pinpoint pattern arrays on the substrate.

Poster Presentation : **MAT.P-748**

Material Chemistry

Zoom 18 FRI 16:00~17:00

The Synthesis and Characterization of Diketopyrrolopyrrole Based Biocompatible Aggregation-Induced Emission Nanoparticles Encapsulated in Pluronic F-127 / PMMA

Geonho Lee, Sang Yoon Lee¹, Seong Hyun Jang, Jun Choi^{2,*}

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²*Korea Institute of Industrial Technology, Korea*

Aggregated-induced emission (AIE) dyes compared to practical commercial fluorescent dyes, have the property of increasing fluorescence at high concentrations. Because of its property, these AIE dyes have potential applications in fields such as chemical sensing, organic light emitting diodes (OLEDs), organic photovoltaics (OPVs), bio-sensing and bio-imaging. In particular, in order to be used in the field of bioimaging, the stability and photoluminescence intensity of dyes are very important. However, the stability of dye molecules increases when aggregates formed by intermolecular forces, but the intensity of fluorescence decreases. In this study, in order to synthesize a highly stable AIE dye, a high durability diketopyrrolopyrrole core based AIE dyes using the triphenylamine derivatives were synthesized, and these dyes showed AIE behavior. Since the synthesized AIE dye does not disperse well in an aqueous environment, and also may negatively affect cell viability, water-dispersible AIE nanoparticles (NPs) using biocompatible polymer Pluronic F-127 and PMMA were synthesized. Various fluorescence intensities were observed according to the content of synthesized dyes, polymers, and surfactants, AIE NPs with excellent particle shape and fluorescence intensity were synthesized by optimizing the content of each component.

Poster Presentation : **MAT.P-749**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Hydrodeoxygenation of Methyl Palmitate over Highly Dispersed Pd Nanoparticles Supported on Hierarchically Porous Carbon Synthesized Using Nanocrystalline Zeolite Templates

JinJu Han, Kyoungsoo Kim^{1,*}

Jeonbuk National University, Korea

¹*Department of chemistry, Jeonbuk National University, Korea*

Hydrodeoxygenation is a key reaction in the upgrading process of bio-fuel. We synthesized hierarchically porous carbon-supported palladium catalyst for the hydrodeoxygenation of methyl palmitate (MP). The carbon support was prepared using ethylene and nanocrystalline beta zeolite as a carbon source and sacrificial template, respectively. The templating synthesis allowed nanocrystalline beta zeolite to inherit its hierarchical pore system composed of zeolite micropores and intercrystalline mesopores to the carbon support. Thus, the carbon structure consisted of ordered micropores with 1-nm diameter and 10 – 40 nm mesopores. All the pores were three-dimensionally connected with each other. Very high surface area (2130 m² g⁻¹) and uniform micropores of the carbon made palladium nanoparticles highly dispersed in a diameter of approximately 1 nm. The hydrodeoxygenation reaction was carried out using semi-batch reactor with constant H₂ pressure of 20 bar. The catalyst exhibited high yield of hydrocarbon in diesel range as compared to commercial Pd/C. The high diesel selectivity was more pronounced at 360 °C. The results were attributed to synergetic combination of the high dispersion of Pd nanoparticles and facile diffusion of heavy reactant molecules through the mesopores. Notably, the hierarchically porous carbon-supported catalyst showed better recyclability than Pd/C. It was confirmed that the palladium nanoparticles confined in the micropores had high stability against particle sintering by transmission electron microscopy observation.

Poster Presentation : **MAT.P-750**

Material Chemistry

Zoom 18 FRI 16:00~17:00

Fabrication of Water-Repellent Platinum(II) Complex-Based Photon Downshifting Layers for Perovskite Solar Cells by Ultrasonic Spray Deposition

Eunhye Hwang, Tae-Hyuk Kwon*

Department of Chemistry, 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

1. Tai, Q.; Tang, K.-C.; Yan, F. *Energy Environ. Sci.* **2019**, 12, 2375
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

Poster Presentation : **MAT.P-751**

Material Chemistry

Zoom 19 FRI 15:00~16:00

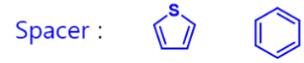
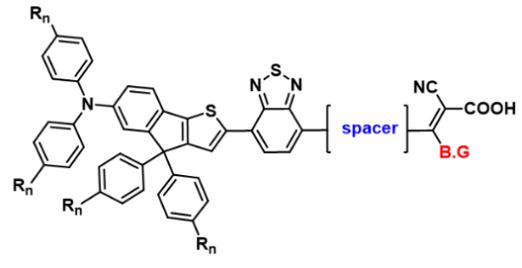
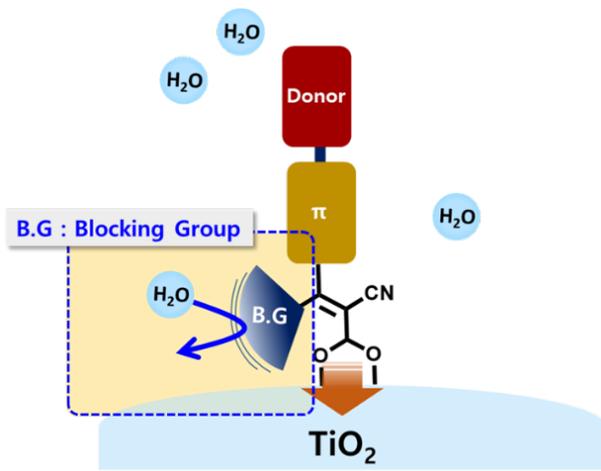
Preventing Degradation and Desorption of Photosensitizer in Aqueous Condition for various Applications

JeongKyeong Lee, Tae-Hyuk Kwon^{1,*}

chemistry, Ulsan National Institute of Science and Technology, Korea

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

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. 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 photoelectrochemical cell(DSPEC) and dye sensitized solar cells(DSSCs) with long term stability.



Poster Presentation : **MAT.P-752**

Material Chemistry

Zoom 19 FRI 15:00~16:00

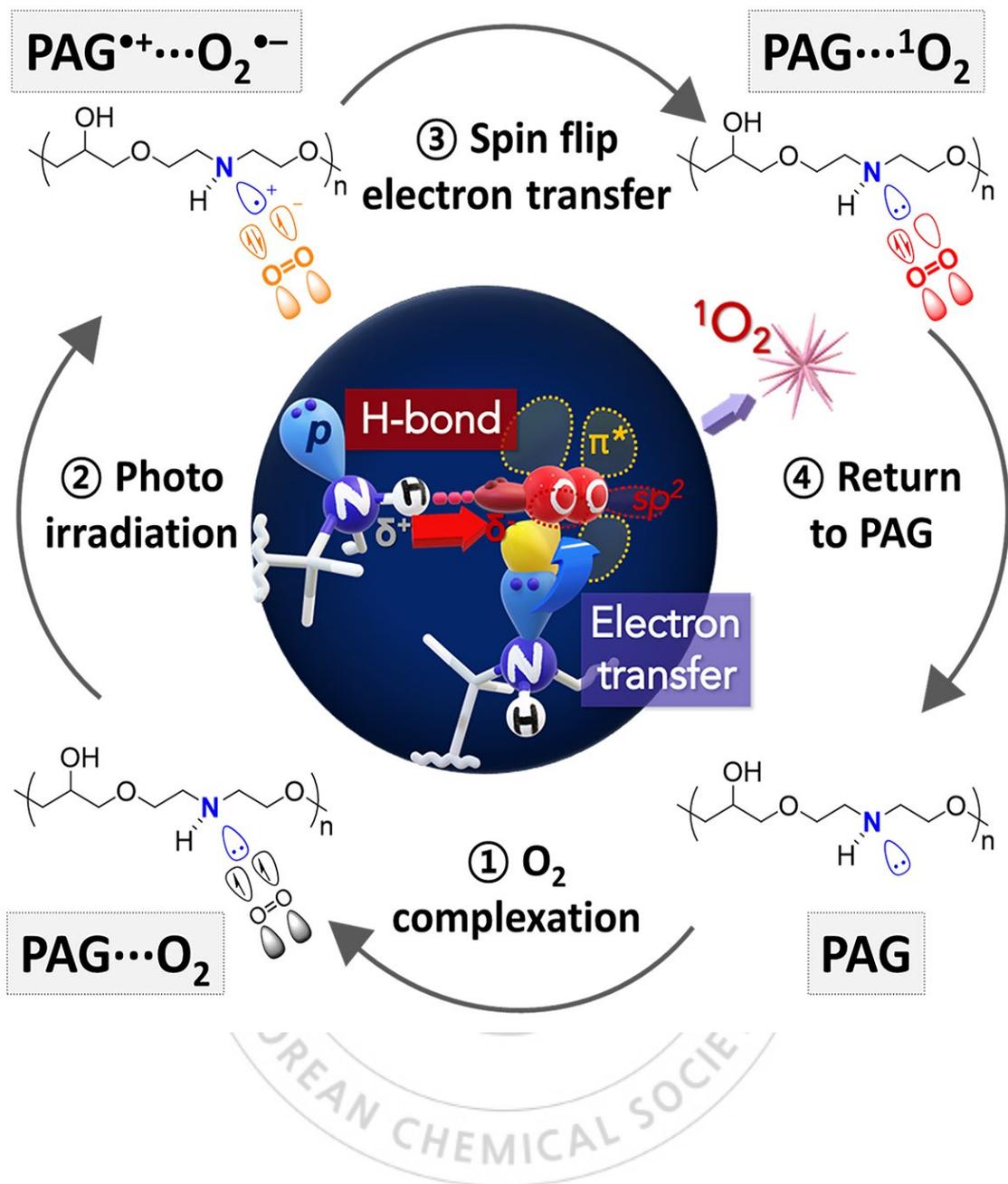
Singlet Oxygen Generation Using Polyaminoglycerol by Spin-Flip Electron Transfer

Jung Seung Nam, Seung Kyu Min^{*}, Byeong-Su Kim^{1,*}, Tae-Hyuk Kwon^{*}

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

¹Department of Chemistry, Yonsei University, Korea

Reactive oxygen species (ROS) have drawn attention owing to their strong oxidation capability. Especially, the singlet oxygen ($^1\text{O}_2$) produced by energy transfer is the predominant species for controlling oxidation reactions efficiently. However, a narrow perspective on the energy transfer (distal pathway) to increase $^1\text{O}_2$ generation could cause the following issues in the developed $^1\text{O}_2$ generator: (i) poor solubility, (ii) low stability or (iii) lack of compatibility. Herein, we introduce a new type of $^1\text{O}_2$ generator based on an aliphatic polyaminoglycerol (PAG), which relies on 'spin-flip electron transfer (proximal pathway)'. The lone pair electron of the nitrogen atom on the PAG backbone and polymer network with hydrogen donor affords strong interaction with O_2 , leading to direct electron transfer to form $\text{PAG}^{\bullet+}\text{-O}_2^{\bullet-}$ under photo-irradiation. Subsequent internal conversion generates $^1\text{O}_2$, and the proximal pathway is demonstrated by a series of photophysical, electrochemical, and computational analyses. The $^1\text{O}_2$ generator, PAG, is successfully employed as photodynamic therapy and antimicrobial reagent.



Poster Presentation : **MAT.P-753**

Material Chemistry

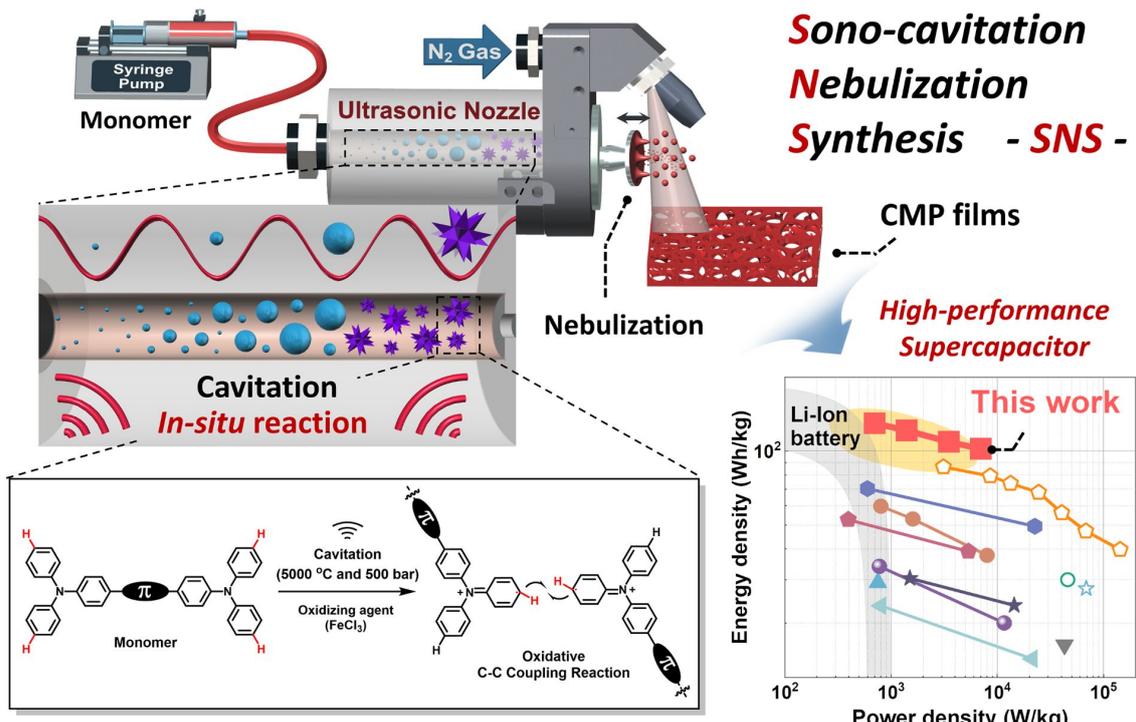
Zoom 19 FRI 15:00~16:00

Sono-Cavitation and Nebulization based In-Situ C–C Coupling of Conjugated Microporous Polymers

Deok-Ho Roh, Tae-Hyuk Kwon*

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

Conjugated microporous polymers (CMP) are prospective energy-storage materials owing to their rigid and cross-linked microporous structures. However, the fabrication of nano- and microstructured CMP films for practical applications is currently limited by processing challenges. We report combined sono-cavitation and nebulization synthesis (SNS) as an effective method for the in-situ synthesis of CMP films from a monomer precursor solution. Using the SNS, simultaneous oxidative C–C coupling polymerization and CMP film fabrication can be achieved. The reaction yield, porosity, and electrochemical properties of the prepared CMP films strongly depend on the applied ultrasonic frequency (120 and 180 kHz). Furthermore, we prepare highly conductive, three-dimensional porous electrodes by layer-by-layer sequential deposition of CMP and single-walled carbon nanotubes through the SNS. The resultant CMP-based symmetric supercapacitors shows high specific capacitances of 755.7 F/g and 61.3 mF/cm² at 10 mV/s. Furthermore, an asymmetric supercapacitor comprising a nano/microstructured CMP cathode and carbon anode achieves an unprecedented high energy (94–130 Wh/kg) and power density (700–14000 W/kg) with a wide working potential window (0–1.4 V) and robust cycling stability of 94.4% retention after 10,000 cycles.



Poster Presentation : **MAT.P-754**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Gold Nanorod – DMSO based PCR array on Foot-and- Mouth Disease Virus Detection

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¹*BioNanotechnology Research Center, Korea Research Institute of Bioscience & Biotechnology, Korea*

Recently, reports have shown that polymerase chain reaction (PCR) can significantly improve performance with the addition of gold nanoparticles (AuNPs). The excellent heat transfer and surface characteristics of nanoparticles should be the main factor to improve PCR efficiency. However, the concentration, shape, and surface functionality of AuNPs affect the results of PCR under normal amplification conditions. In this work, we describe the performance of PCR using Au nanorod (AuNR) and DMSO for sensitive and rapid detection of foot-and-mouth disease viruses (FMDVs). Foot-and-mouth disease (FMD) is an acute infection of hoof livestock with a fatality rate of 5 to 55%. Since there is no special treatment, it can cause serious damage to the hoof livestock industry. Therefore, for fast and sensitive FMDV detection, it is necessary for better detection techniques than before. Our results show that the detection limit of real-time improved with AuNR and DMSO. Furthermore, the detection time of FMDVs can be reduced depending on the amount of AuNR and DMSO. Our sensitive and specific nano-PCR systems can improve the quality and productivity of PCR assays, and should be useful for diagnosing early FMDV infections.

Poster Presentation : **MAT.P-755**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Facile synthesis of mesoporous TiO₂ film with high surface area through a dual-templating method for the electron transport layer of perovskite solar cells

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In perovskite solar cells (PSCs), TiO₂ layer plays a crucial role as an effective scaffold for loading perovskite materials and separating charge carriers generated in the perovskite. The mesoporous structure of the TiO₂ layer is well known to enhance the power conversion efficiency of PSCs. Here, we reported a facile route to synthesize mesoporous TiO₂ film using both triblock copolymer surfactant and phenolic resin as templates. The film was simply prepared through spin coating of an ethanol solution including titanium isopropoxide, polymer surfactant F-127, phloroglucinol and formaldehyde. The coated solution was converted to a mesostructured nanocomposite film of titania oligomer, phenolic resin and surfactant via a solvent evaporation-induced self-assembly process. In the subsequent air calcination process at 500 °C, TiO₂ frameworks were crystallized, and the surfactant and the resin were removed to form mesopores. The PSC fabricated with the obtained TiO₂ film exhibited power conversion efficiency of 6.44 %, which is higher than the value of the PSC composed of commercial TiO₂ film. The surface areas of the powder-form samples, characterized by N₂ adsorption, revealed that the result was attributed to the high surface area accommodating the large amount of perovskite nanocrystals. The mesoporous TiO₂ had the Brunauer-Emmett-Teller (BET) surface area of 125 m² g⁻¹, whereas the commercial TiO₂ was 38 m² g⁻¹. Such a high surface area resulted from synergistic effect of surfactant and phenolic resin template. They prevent the collapse of mesopores during the crystallization. TiO₂ film synthesized using the only surfactant exhibited the BET surface area of 80 m² g⁻¹. The result of comparative synthesis indicates that the dual-templating system is effective to form a mesostructured TiO₂ with high surface area.

Poster Presentation : **MAT.P-756**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Effect of zeolite crystal thickness and mesopore architecture on dynamic adsorption/desorption characteristics for p-xylene

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Volatile organic compounds (VOCs) resulted from human activities are toxic air pollutants, leading to severe health problems. With continuous industrial development, the VOC emission amount increases tremendously every year. Zeolites have been widely used as adsorbents with their attractive physicochemical properties (i.e. high surface area, crystalline structure) for VOC adsorptions. However, severe diffusion limitation causes a decrease in the adsorption capacity of zeolites for VOCs. Here, we report an effect of zeolite crystal thickness and mesopore architecture for p-xylene adsorption. Several MFI-type zeolites with various crystal sizes, ranging from 300nm to 2nm (i.e. from bulk to nanosheet) were prepared through hydrothermal synthesis procedure, using different structure-directing agents to investigate the crystal thickness effect. Also, MFI zeolite having different mesopore openings (i.e. open mesopore, constricted mesopore) were synthesized for studying the effect of architecture via post-synthetic desilication. By varying the particle size, the breakthrough time of MFI zeolite was increased up to 2.3 times as their thickness becomes smaller. The increase in breakthrough time can be attributed to shortening the diffusion path length and expanding the external surface area by decreasing crystal size. In the case of the mesopore architecture effect, constricted mesopore show slower mass transfer because their mesopores are not connected to the outside. In contrast, there is no mass transfer decline in the opened mesopore. Besides, MFI zeolite having opened mesopore type gave desorption at lower temperatures as compared to constricted mesopore type.

Poster Presentation : **MAT.P-757**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Brimonidine-Montmorillonite Hybrid for Ocular Drug Delivery System

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Brimonidine (BMD) is often prescribed as an eye drop to reduce the intraocular pressure (IOP) for glaucoma treatment. However, eye drops are limited by rapid clearance from the precocular surface, and hence a low ocular drug bioavailability. Therefore, in this study, we propose montmorillonite (MMT), as a delivery carrier, hybridized with BMD (BMD–MMT) for topical drug delivery to the eye. The BMD–MMT hybrid was prepared by intercalating the BMD molecules in the interlayer space of the MMT lattice via ion-exchange reaction; it was then formulated with polyvinyl alcohol (PVA) to produce a dry tablet (i.e., BMD–MMT@PVA). The BMD–MMT@PVA hybrid drug released BMD in a sustained manner for more than 5 h under in vitro conditions. When the hybrid drug was administered to rabbit eyes in vivo, 43% and 18.5% BMD–MMT still remained on the precocular surface for 10 and 60 min after administration, respectively. Thus, the BMD–MMT@PVA hybrid drug exhibited a prolonged decrease in IOP, that is, for 12 h, which was approximately two times longer than that observed with the commercially available BMD eye drop, Alphagans P.

Poster Presentation : **MAT.P-758**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Niclosamide-Montmorillonite/Tween60 Ternary Hybrids with Enhanced Bioavailability Towards Covid-19 Treatment

Seungjin Yu, Huiyan Piao¹, Sanoj Rejinold Nirichan¹, Geunwoo Jin², Goeun Choi^{3,*}, Jin-Ho Choy^{4,*}

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Niclosamide (NIC), a conventional anthelmintic agent, is emerging as a repurposed drug for the Covid-19 treatment. The clinical efficacy was, however, very limited due to its low oral bioavailability resulting from its poor aqueous solubility. In the present study, a new hybrid drug delivery system made of NIC, montmorillonite (MMT), and Tween 60, is proposed to overcome this obstacle. At first, NIC molecules were immobilized into the interlayer space of cationic clay, MMT, to form NIC-MMT hybrid, which could enhance the solubility of NIC, and then the polymer surfactant, Tween 60, was further coated on the external surface of NIC-MMT to improve the release rate and the solubility of NIC, and eventually the bioavailability under gastrointestinal condition when orally administered. Finally we have performed an in-vivo pharmacokinetic study to compare the oral bioavailability of NIC for the Tween 60 coated NIC-MMT hybrid and was compared with the Yomesan®, a commercially available NIC. Exceptionally, the Tween 60 coated NIC-MMT hybrid showed higher systemic exposure of NIC than Yomesan®. Therefore, the present NIC-MMT-Tween 60 hybrid can be a potent NIC drug formulation with enhanced solubility and bioavailability in-vivo for treating Covid-19.

Poster Presentation : **MAT.P-759**

Material Chemistry

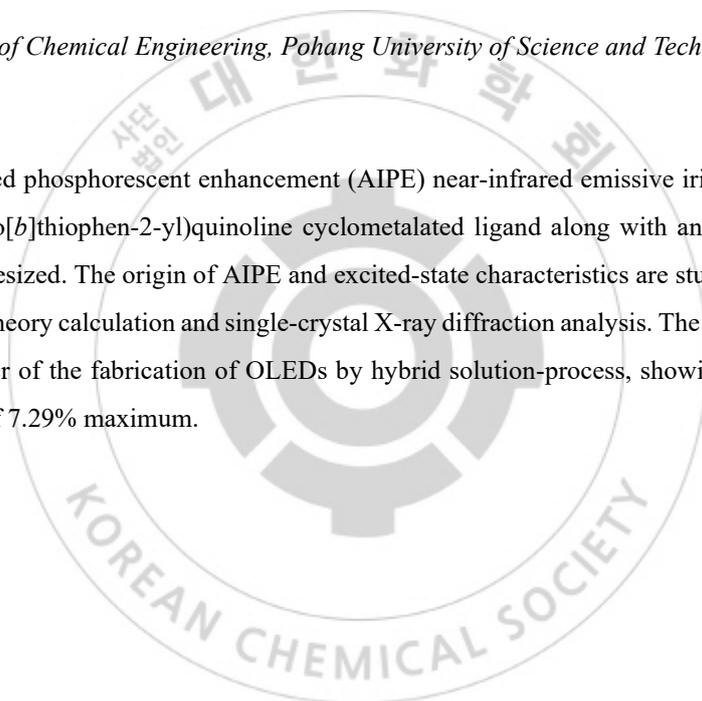
Zoom 19 FRI 15:00~16:00

Aggregation-Induced Near-Infrared Emission of Ir(III) Organometallic Phosphorescent Materials

Hae Un Kim, Dohyun Kim, Taiho Park*

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

Aggregation-induced phosphorescent enhancement (AIPE) near-infrared emissive iridium(III) complexes containing a (benzo[*b*]thiophen-2-yl)quinoline cyclometalated ligand along with ancillary picolinate are designed and synthesized. The origin of AIPE and excited-state characteristics are studied with the help of density functional theory calculation and single-crystal X-ray diffraction analysis. The complexes are doped in the emitting layer of the fabrication of OLEDs by hybrid solution-process, showing external quantum efficiency (EQE) of 7.29% maximum.



Poster Presentation : **MAT.P-760**

Material Chemistry

Zoom 19 FRI 15:00~16:00

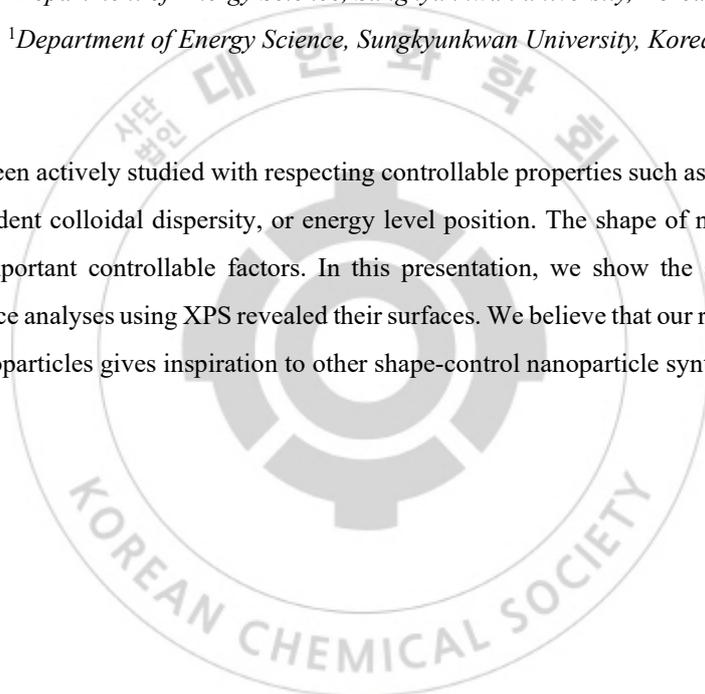
Shape-controlled colloidal InP quantum dot

Youngsik Kim, Sohee Jeong^{1,*}

Department of Energy Science, Sungkyunkwan university, Korea

¹*Department of Energy Science, Sungkyunkwan University, Korea*

Quantum dot has been actively studied with respecting controllable properties such as size-dependent band gap, surface-dependent colloidal dispersity, or energy level position. The shape of nanocrystals could be also one of the important controllable factors. In this presentation, we show the shape-controlled InP nanocrystals. Surface analyses using XPS revealed their surfaces. We believe that our research on the shape-controlled InP nanoparticles gives inspiration to other shape-control nanoparticle synthesis research.



Poster Presentation : **MAT.P-761**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Synthesis of Au/Ag Ring-in-a-triangle Nanoframes having Quad-holes Hotspots with Stable SERS Signal

Sungeun Go, Sungho Park*

Department of Chemistry, Sungkyunkwan University, Korea

For obtaining high resolution of surface enhanced Raman scattering (SERS) signal, hotspots are essential. In case of nanostructures, hotspots are usually generated where the electromagnetic field is extremely concentrated, such as a sharp tip or narrow gap. Especially, novel metal nanoframes having intra-hotspots attracted much attention because even a single particle exhibits SERS activity. Noble metal have great SERS effect due to their unique localized surface plasmon resonance (LSPR) properties. Among them, Au/Ag alloy nanoparticles have exhibited both stability and high SERS sensitivity. In this paper, we synthesize ring-in-a-triangle nanoframes (RITs) by stepwise synthetic process. The platinum frame acts as a skeleton, and gives structural stability. By concentric growth of gold and silver, triangle frame and the inscribed circle generate hole-shaped hotspots at regular intervals which called quad-hole hotspots (QH hotspots). Depending on the amount of added Au^{3+} and Ag^+ ions, the size of QH hotspots can be easily controlled from 20nm to 5nm. QH hotspots have largely enhanced electromagnetic field due to lightening rod effect of triangle and plasmonic coupling effect in randomly alloyed nanohole close to the tip. Through comparison with the single triangular nanoframes on the substrate, we can confirm that QH hotspots improve the SERS intensity by 4 times. Also, assembled RITs substrate can be considered as nanoporous substrate. These unique nanoparticles serve as excellent substrate for SERS based biosensing platform.

Poster Presentation : **MAT.P-762**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Oxidative dehydrogenation of ethane in CO₂ using Cr-TUD-1 Catalyst

Numan Muhammad, Changbum Jo^{*}, Sang-Eon Park^{*}

Department of Chemistry and Chemical Engineering, Inha University, Korea

Ethane oxidative dehydrogenation in the presence of CO₂ as soft oxidant was studied over the Cr-TUD-1 catalyst, having a nanosponge structure with a surface area of ~ 650 m² g⁻¹. In Cr-TUD-1 support, Cr⁶⁺ species were well distributed in form of monochromate. During ethane dehydrogenation in N₂ atmosphere, Cr⁶⁺ suffer with partial reduction to Cr³⁺/Cr⁰, that is responsible in formation of large-sized Cr₂O₃ and Cr_x particles. Due to coke formation and chromium sintering, the Cr-TUD-1 catalyst was deactivated within 2 h. Altering N₂ flow with CO₂ enhanced the catalyst stability and produced diminutive coke, that was attributed to enhanced inter-convertibility of Cr⁶⁺ and highly dispersed Cr³⁺ as well as a reverse Boudouard reaction between coke and CO₂ resulting in coke removal. Also, it was observed that large Cr₂O₃ nanoparticles could not be readily oxidized to Cr⁶⁺ by CO₂. The stability of catalyst was further enhanced with addition of O₂ to CO₂. The oxygen contributed to the redispersion of sintered Cr₂O₃ nanoparticles to form isolated Cr⁶⁺ species that are the active sites for ethane dehydrogenation.

Poster Presentation : **MAT.P-763**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Effects of Graphene Oxide-Gold Nanoparticle Nanocomposite on Highly Sensitive Foot-and-Mouth Disease Virus Detection

Jong-won Kim, Chang-Soo Lee^{1,*}

Bionanotechnology Research Center, Korea Research Institute of Bioscience & Biotechnology, Korea

¹*BioNanotechnology Research Center, Korea Research Institute of Bioscience & Biotechnology, Korea*

The polymerase chain reaction (PCR) has become one of the powerful molecular diagnostic techniques for last decades, nevertheless, it has been still frequently impaired by its low specificity, poor sensitivity and false positive results. Recently, nanomaterials, including metal nanoparticles, carbon nanomaterials, quantum dots and metal oxide, have been widely reported to affect the PCR with improvement of both quality and productivity of PCR assay. Here, we present nanomaterial-assisted PCR (nano-PCR) using a nanocomposite (GO-AuNPs) composed of graphene oxide (GO) and gold nanoparticles (AuNPs) for highly sensitive detection of foot-and-mouth disease virus (FMDV). GO and AuNPs have been widely served as biomedical materials for diagnosis, therapy and drug delivery due to their unique chemical and physical properties. The foot-and-mouth disease (FMD) is a highly contagious and fatal disease in cloven-hoofed animals, thus bringing about a serious damage to the swine industry. Therefore, a highly sensitive and specific method has been required for the efficient detection of FMDV. The detection limit of real-time PCR improved by ~1,000 fold when assisted by GO-AuNPs. We also designed a system of detecting serotypes in a single assay based on melting temperatures. This sensitive and specific nano-PCR system can be effectively used for clinical diagnosis of early FMDV infection, thus, expecting a useful application prospects in biomedical field.

Poster Presentation : **MAT.P-764**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Metal Frame-based Ligand Modification Control for Selective Oriented Gold Nanocube Assembly for Reproducible SERS with Narrow Distribution

Kyunjong Sim, Jwa-Min Nam*

Department of Chemistry, Seoul National University, Korea

Surface-enhanced Raman scattering (SERS) is a commonly used sensing technique and its signal intensity is affected by the intensity of localized electromagnetic (EM) fields that arise from plasmon excitation in plasmonic nanoparticles. In addition, the formation of nanogap or junction between nanoparticles can generate higher SERS signal than single nanoparticle due to hotspots, which are regions of highly localized EM fields. It means that nanogap or junction structures play an important role in signal reproducibility and distribution. So, precisely controlled plasmonic nanostructures in a high yield are needed for obtaining strong and reproducible SERS signals with narrow distribution. In general, the assembled structures of gold nanospheres can form almost similar nanogaps between particles due to isotropic structure of spheres. On the other hand, the assembly of anisotropic nanoparticles such as nanocube results in different signal reproducibility because various nanogap structures (e.g., face-to-face, face-to-edge, and edge-to-edge) can be formed. In order to reproducible SERS signal with narrow distribution, a strategy is needed for obtaining precisely controlled assembly structures with uniform nanogaps. Here, we have successfully synthesized site-selective DNA-modified gold nanocube through metal frame-based ligand modification method. The structure and optical properties of various nanocube assemblies were investigated and the correlation between them was analyzed. Our modification strategy provides new platforms in precisely forming plasmonic assembled structures with uniform nanogaps for reproducible SERS application.

Poster Presentation : **MAT.P-765**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Concentric Nanorings with Intertwined Triple-Rings: The Outer Ring enhances Electric Near-Field Focusing between Core and Second Rings

Sungjae Yoo, Sungho Park*

Department of Chemistry, Sungkyunkwan University, Korea

Designing the complex plasmonic nanoframe structures is of great significance to effectively improve the interaction between light and nanoparticles, but it remains a significant challenge due to low controllability of the synthetic strategy in the solution phase. In this paper, we design the nanorings with intertwined triple-rings that three nanorings with different diameters are arranged within a single nanostructure for significantly amplifying the efficiency of the near field focusing. The resulting nanorings with intertwined triple-rings can be realized through rational multi-stepwise reactions including selective etching of Au, overgrowth of Au, selective deposition of Pt, and well-faceted concentric growth of Au, and concentric growth of Au. Unique localized surface plasmon resonance (LSPR) coupling characteristics are systematically studied. Typically, through synergy effect of each nanorings (e.g., outer, middle, and core ring act as light absorber, gap controller, and near field enhancer, respectively), Au nanorings with intertwined triple-rings can effectively generate the strong electric near-field confinement effects in a single entity, resulting in high-resolution of Raman signals of adsorbed molecules in nanogaps. Remarkably, the measured enhancement factors have approximately two-order magnitude enhancement value (1.3×10^9) compared to that of double nanoring with different geometries (7.8×10^7 and 2.6×10^7).

Poster Presentation : **MAT.P-766**

Material Chemistry

Zoom 19 FRI 15:00~16:00

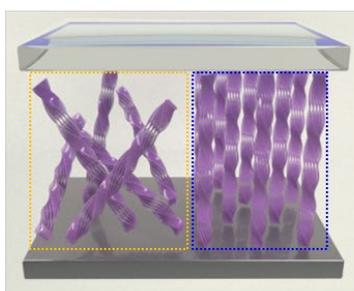
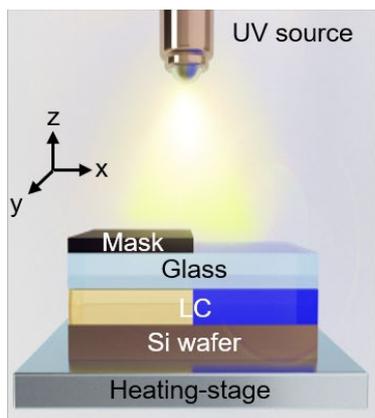
Study on the 3D nanopatterning with photo-responsive liquid crystal molecules for use as a chiral photonic crystal

Wongi Park, Dong Ki Yoon^{1,*}

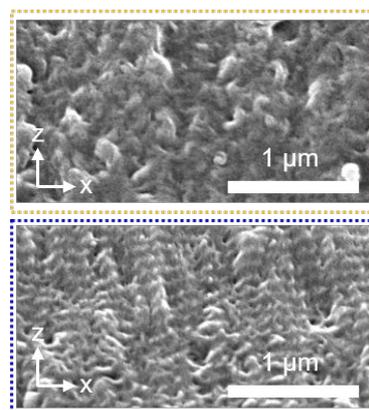
*Graduate School of Nanoscience and Technology, Korea Advanced Institute of Science and Technology,
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Chiral photonic crystal (PC), which has a periodic chiral nanostructure with differing refractive indices, has many interesting chiro-optical properties, such as light manipulation with its propagation and polarization. As those can directly be used in our daily lives, for example, color filter, sensor, security and smart window, 3D nanopatterning to fabricate the chiral PC has been considered essential research topics. Among many methods to realize this, chiral liquid crystal (LC) phases, such as the cholesteric (CLC) phase and blue phase (BP), show many advantages in the fabrication process as they spontaneously form the chiral nanostructures in a specific temperature range. However, as those LC phases are more like liquid phase and show thermally and mechanically poor stability, additional stabilization processes are required. In this research, we reported a new method to fabricate the chiral PC more simply with enhanced stability. The helical nanofilament (HNF) phase, made of bent-shaped LC molecules, shows solid-like material properties and is thermally and mechanically stable. Moreover, as its helical pitch is in a sub-hundred-nanometer scale, HNF can be used as chiral PC if uniaxially oriented. We developed a new method to uniaxially orient the HNFs in a large area with the photoalignment method by incorporating azobenzene moieties with LC molecules. Based on this simple method, chiral PC was easily fabricated and show many useful applications such as sensors, security code, and color filter.



- Shadowed area
- UV shined area



Poster Presentation : **MAT.P-767**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Core-shell structural LTO/C composites derived from Ti-based metal-organic framework: the application as anode materials for lithium secondary batteries

Tae Woo Kim^{*}, Hyunuk Kim

Energy Materials Laboratory, Korea Institute of Energy Research, Korea

One of the most promising anode material candidates for Li secondary batteries is lithium titanium oxides, $\text{Li}_4\text{Ti}_5\text{O}_{12}$ (LTO). Although it has a lower specific capacity of approximately 175 mAh/g than does graphite (372 mAh/g), this material shows the unique property of the negligible lattice change in the Li-ion insertion/desertion process, providing excellent high-rate cycling stability. The biggest obstacles of limiting the application of LTO material electrodes are poor electrical conductivity and low lithium-ion diffusion coefficient. To overcome these problems, in this work carbon-coated LTO (LTO/C) composites with the core-shell-type structure are synthesized and it is derived from Ti-based metal-organic framework (Ti-MOF). For the synthesis of the LTO/C composites, Ti-MOF was chemically lithiated by n-BuLi and heated at different temperatures (500-800 °C) in an inert atmosphere. According to powder X-ray diffraction analysis, the as-lithiated sample shows an amorphous structure, and the LTO structure is generated after heat-treatment of above 600 °C. Transmission electron microscopy clearly shows core-shell-type LTO particles surrounded by carbon layers with a thickness of 3-5 nm. The electrochemical measurements clearly demonstrate the promising functionality of the present LTO/C composite as anode for lithium secondary batteries. The LTO/C composite obtained by heating at 700 °C show the largest discharge capacity (cal. 152 mAh/g) with good cyclability. The present experimental findings underscore the validity of the use of MOF as a useful platform for new synthetic strategies of carbon coated LTO materials and also for the improvement of their functionality.

Poster Presentation : **MAT.P-768**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Fabrication of Self-assembly Templates using Liquid crystal Topological Defects

Geonhyeong Park, Dong Ki Yoon^{1,*}

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

Most defects are regarded as beings that must be eliminated in order to improve their properties and efficiency in most materials science. However, recently, there are some efforts to regularly control the defect structure itself in the liquid crystals. This defect engineering with liquid crystals is drawing attention because it can be applied to various scaffolds for lithography, polymer actuators, controlling living matter, particle trapping, 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 regularly controlled the more complex defect structures by using the appropriate confinement effect and the intrinsic elasticity of the liquid crystal. These unique defect structures are expected to be used as a template to assemble various organic molecules such as small molecules, supramolecules, and polymers, which are advanced templates than previously reported

Poster Presentation : **MAT.P-769**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Maximizing Plasmonic Effect in Multi-metallic Nanostructures

Hyosun Lee

Korea Institute of Industrial Technology, Korea

Utilizing solar energy for chemical reaction have has received huge attraction to overcome the limitation of conventional thermal catalytic reaction. Recently, it has been reported that plasmoninduced energetic hot electrons transfer to reactant molecules on the metal surface and activate the molecular orbitals of adsorbates or metal-adsorbate complexes, resulting in enhancement of reactivity and selectivity. However, it remains challenging because plasmonic noble metals enabling efficient absorption of light in UV-Visible range have inherently insignificant catalytic properties. Therefore, multi-metallic plasmonic catalytic architectures integrating the plasmonic metal with the catalytic metal has required as a new direction to open the possibility for increasing the reaction activity further in photo-assisted catalytic reaction. In this study, we develop dilute Pd/Au alloys where single- or multiisolated Pd atoms are decorated on the surface of Au nanoparticles with different concentration. We also investigate the optimized structure of multi-metallic nanoparticles to maximize the effect of surface plasmon on chemical reaction. This study has been conducted with the support of the Korea Institute of Industrial Technology as "Production technology creative research project (KITECH EI-21-0016)".

Poster Presentation : **MAT.P-770**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Study of Spectral Bandwidth and Vibronic Transitions Based on the Molecular Design of Azaacene-based Narrowband Green-emitting Fluorophores

Jung Min Ha, Sungnam Park*, Han Young Woo*

Department of Chemistry, Korea University, Korea

To investigate the design protocol for the pure-green-emitting fluorophores, three molecules (DBBNP, DBBNP2CN1, and DBBNP2CN2) based on the tetraazaacene core with different positions of cyano groups were synthesized. According to density functional theory (DFT) calculation at B3LYP level, reduced charge transfer character and Huang-Rhys factor (FRF) at higher frequency of vibronic transitions could be obtained from DBBNP2CN2. The spectroscopic data also support that DBBNP2CN2 shows the narrowest PL emission with discrete vibronic structures in various solution and film state. Interestingly, the intensity ratio of ν_{0-1} and ν_{0-0} (I_{0-1}/I_{0-0}) vibronic transitions of DBBNP2CN2 (0.67) was smaller than that of DBBNP (1.13) or DBBNP2CN1 (0.80). The organic light-emitting diode employing DBBNP2CN2 shows narrower green EL emission at 518 nm with smaller bandwidth (50 nm) than those of the devices fabricated with DBBNP (81 nm) or DBBNP2CN1 (99 nm). Our work to control the HRFs of the vibronic peaks by modulation of the molecular structures enables us to achieve narrow emission bandwidth with less I_{0-1}/I_{0-0} , suggesting the logical design strategy for fluorescent organic emitters and contributes to meet the growing demands for high-resolution display and its wide color gamut..

Poster Presentation : **MAT.P-771**

Material Chemistry

Zoom 19 FRI 15:00~16:00

Alkyl Side Chain Engineering of IDT Based Non-Fullerene Acceptors for High Performance Organic Solar Cells

Young Wan Lee, BongSoo Kim*

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

IEHICO-4F is a known high-performance and near-IR absorption contained non-fullerene acceptor (NFA) molecule. Energy levels of IEHICO-4F is well-matched with p-type polymer PTB7-Th, which makes low voltage loss (~0.5 V) and efficient exciton separation in bulk-hetero junction organic solar cells (BHJ-OSCs). However, there are few reports about specific effect of alkyl chains in the IEHICO-4F molecules. Therefore, we have synthesized IRICO-4F derivatives, where 'R' is respective alkyl chains i.e., ethylbutyl (EB), ethylhexyl (EH), octyl (O) and decyl (D) for IEBICO-4F, IEHICO-4F, IOICO-4F and IDICO-4F, respectively. The OSCs device with PTB7-Th and branched alkyl side chain contained IEBICO-4F and IEHICO-4F showed PCE 10.63% and 10.64%. However, linear side chain having IOICO-4F and IDICO-4F blend films showed PCE 9.93% and 8.98%. These results suggest that IRICO-4F with branched alkyl chain (EB and EH) shows higher performance than IRICO-4F with linear alkyl chain (O and D). For stability issue, proper alkyl chain length has more relationship than branch factors. To understand how alkyl chain affects the OSCs results, morphological analysis with Atomic force microscope (AFM), Grazing incidence Wide Angle X-ray Scattering (GIWAXS) and Transmission Electron Microscope (TEM) were followed. This work provides reasonable strategies to design NFA molecules.

Poster Presentation : **ELEC.P-772**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Poly(vinyl carbazole) as a high energy and power density cathode material for Mg-based dual ion battery

Amol Bhairuba Ikhe, Myoungho Pyo*

Department of Printed Electronics Engineering, Suncheon National University, Korea

The next-generation secondary batteries based on earth-abundant elements are in high demand. Magnesium metal or magnesium-ion batteries (MIBs) can be an attractive alternative energy storage device due to the earth's abundance of Mg and its high theoretical capacity (3833 mAh/cm³) compared with current lithium-ion batteries (Graphite anode, 850 mAh/cm³). However, the development of electrode materials with higher energy/power densities is arduous for magnesium batteries due to the incompatibility of Mg metal with high voltage electrolytes. Herein, we designate a possible solution that contains alloy-type anodes (3Mg/Mg₂Sn) and high-voltage redox polymer (poly(vinyl carbazole), PVCz) cathodes in Mg(TFSI)₂/acetonitrile (TFSI = bis(trifluoromethanesulfonyl)imide). The PVCz was first potentiostatically synthesized at 1.0 V vs Ag wire and then the obtained low molecular weight PVCz was chemically crosslinked (x-PVCz). The electronic conductivity and the density of micro-to-macro pores were enhanced in x-PVCz, resulting in a high specific capacity (122 mAhg⁻¹) even at a rate of 2000 mA g⁻¹ (14.3C) in a 3-electrode system. This corresponds to energy and power densities of 384 Whkg⁻¹ and 6300 Wkg⁻¹, respectively, which are excellently high values for magnesium batteries. The cyclic stability of x-PVCz was also admirable, delivering 94.2% of the initial capacity through 2000 charge/discharge cycles. Finally, a magnesium-based dual ion battery (MDIB) was assembled using de-magnesiated 3Mg/Mg₂Sn anode and x-PVCz cathodes in Mg(TFSI)₂/acetonitrile electrolyte. The MDIB also retains the unique properties of x-PVCz delivering excellent cyclic stability (97.3% retention during 1000 cycles), high energy density (344 Whkg⁻¹), and power density (5860 Wkg⁻¹). This work proposes that the MDIBs with a cell configuration of D-3Mg/Mg₂Sn | Mg(TFSI)₂/ACN | x-PVCz could be a promising solution to overcome the current deficiencies of magnesium batteries.

Poster Presentation : **ELEC.P-773**

Electrochemistry

Zoom 20 FRI 15:00~16:00

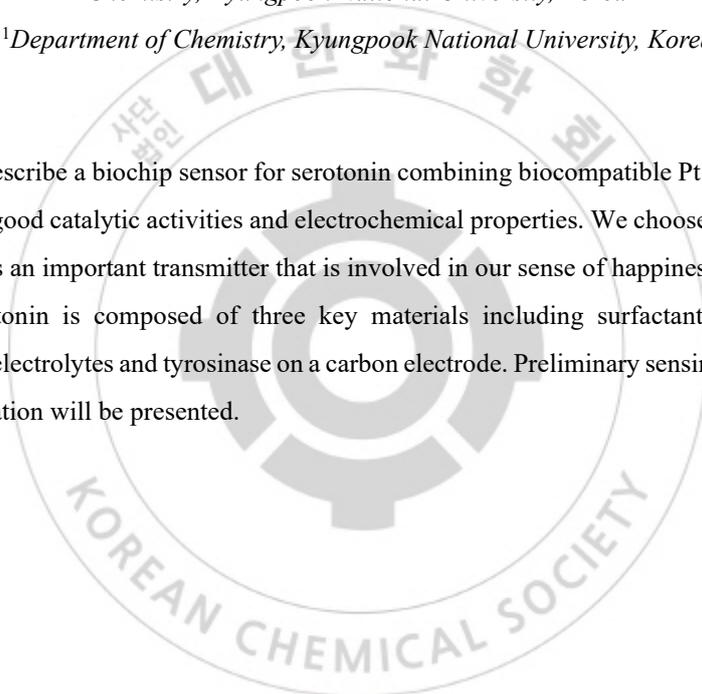
Serotonin detection with Pt nanoparticles incorporated electrodes

Nayeong Ku, Hye Jin Lee^{1,*}

Chemistry, Kyungpook National University, Korea

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

In this poster, we describe a biochip sensor for serotonin combining biocompatible Pt nanoparticles, which are known to have good catalytic activities and electrochemical properties. We choose serotonin as a target analyte because it is an important transmitter that is involved in our sense of happiness. Our amperometric biosensor for serotonin is composed of three key materials including surfactant stabilized platinum nanoparticles, polyelectrolytes and tyrosinase on a carbon electrode. Preliminary sensing results and sensors surface characterization will be presented.



Poster Presentation : **ELEC.P-774**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Fe-Fe₃C Nanoparticles Embedded in Tubular Graphitic Carbon for High-Performance Anode Materials in Sodium-Ion Batteries

Achmad Yanuar Maulana, Da Won Lee, Boram Yun, Jongsik Kim*

Department of Chemistry, Dong-A University, Korea

Sodium-ion batteries (SIBs) presented good prospects in the future compared to lithium-ion batteries (LIBs) due to abundant resources and cheaper price of sodium. Currently, graphite is one of the well-known carbon materials as a commercial anode in LIBs. However, the high irreversible capacity due to the formation of thick SEI layers and the larger radius of sodium (1.02 Å) than lithium (0.76 Å) makes graphite unsuitable for sodium to intercalate through its small interlayer distance. To achieve the maximum potential of carbon anode materials in SIBs, one of the main strategies is focused on fabricating carbon-based materials with various microstructures and strengthening their catalytic reactivity. In this work, the Fe-Fe₃C nanoparticles embedded in tubular graphitic carbon (Fe-Fe₃C@TGC) were synthesized by simple chemical vapor deposition (CVD). The hybridization of Fe-Fe₃C with the tubular carbon facilitates the catalytic reaction to achieve reversible capacities by preventing the excess formation of SEI layers as well as the enhancement of the conductivity. The Fe-Fe₃C@TGC represents enhanced cyclability and high reversible discharge capacity of 376.2 mAh g⁻¹ after 1000 cycles at a current density of 50 mA g⁻¹ as an anode for SIBs.

Poster Presentation : ELEC.P-775

Electrochemistry

Zoom 20 FRI 15:00~16:00

A Study on the improvement of electrochemical performance of Fe₂O₃/N-doped Graphitic Carbon Nanoparticles as an Anode Material for Sodium Ion Batteries

Jungwook Song, Chaeun Lee¹, Jung Hwan Kim¹, Hyunjeong Gim¹, Jongsik Kim^{*}

Department of Chemistry, Dong-A University, Korea

¹*Chemistry, Dong-A University, Korea*

Sodium ion batteries (SIBs) have been gaining attention as an alternative to LIBs due to sufficient resources, low cost and similar redox reaction of sodium compared to lithium. Fe₂O₃ has a high theoretical capacity (1007 mA h g⁻¹), low cost and non-toxic, which aspects are attractive as an anode material in SIBs. However, Fe₂O₃ suffers from low cycle stability and reversible capacity from its low electronic conductivity, volume changes and aggregation during the charge-discharge process. In order to overcome these problems, we synthesized Fe₂O₃/N-doped graphitic carbon (Fe₂O₃/NGC) using dopamine that includes carbon and nitrogen elements. Fe₂O₃/NGC composite showed enhanced capacity retention and a reversible capacity with a discharge capacity of about 502.9 mA h g⁻¹ after 150 cycles at 100.7 mA g⁻¹ and 0.01-3.0 V compared to bare Fe₂O₃. In addition, Fe₂O₃/NGC composite showed the excellent rate capability, for example, the capacities of 159.9 and 122.9 mA h g⁻¹ after 300 cycles at current densities of 1007 (1C) and 2014 (2C) mA g⁻¹. The reversible conversion reaction of Fe₂O₃/NGC during the charge-discharge process was also clearly monitored by the ex-situ XRD, Raman, and TEM analyses.

Poster Presentation : **ELEC.P-776**

Electrochemistry

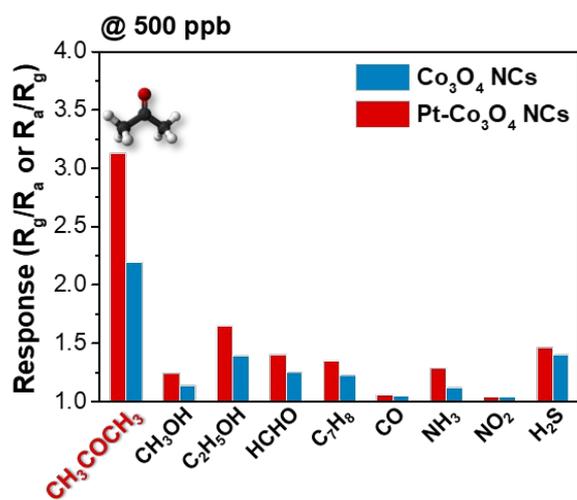
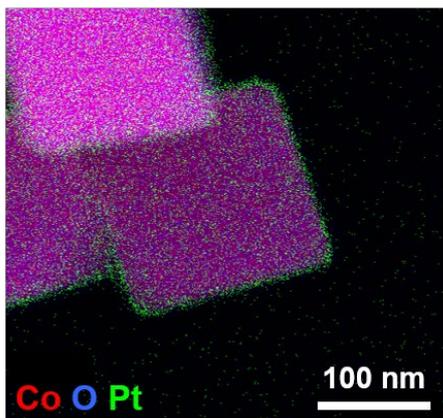
Zoom 20 FRI 15:00~16:00

Facile Photochemical Formation of Pt on Semiconductor Co_3O_4 Nanocubes for the Sensitive Detection of Acetone at the ppb Level

Ahyeon Ma, Ki Min Nam*

Department of Chemistry, Pusan National University, Korea

Pt-supported Co_3O_4 nanocubes (Pt- Co_3O_4 NCs) were prepared by the photodeposition of Pt nanoparticles on Co_3O_4 NCs. The Pt nanoparticles were evenly distributed and well associated with the Co_3O_4 NCs. This facile metal deposition process provides a new opportunity for the fabrication of advanced sensing devices. The Pt- Co_3O_4 NC sensor showed a higher p-type response than those of the other Co_3O_4 sensors in the detection of 500 ppb acetone at 200 °C, with a maximal response (R_g/R_a) of 3.1. Co_3O_4 NCs were found to have a larger neck diameter and hole accumulation layer at the interface than Co_3O_4 nanospheres (Co_3O_4 NSs). In addition, many oxygen species created a thick hole accumulation layer at the surface of Pt- Co_3O_4 NCs because of the spillover effect of Pt nanoparticles. This layer provided a wide channel for charge carriers, resulting in better sensitivity and selectivity of the sensor. Furthermore, the Pt- Co_3O_4 NC sensor works reasonably well under humid conditions and can potentially be applied in aerobic analysis. Thus, the prepared Pt- Co_3O_4 NCs exhibited satisfactory gas-sensing properties for application in healthcare monitoring systems.



Poster Presentation : ELEC.P-777

Electrochemistry

Zoom 20 FRI 15:00~16:00

Sunlight-driven Water Splitting over Perovskite-type BaNbO₂N Photoanodes Prepared by a Polymerized Complex Method

Sohyeon Kim, Jeongsuk Seo*

Department of Chemistry, Chonnam National University, Korea

Hydrogen is an ideal alternative as an eco-friendly, renewable fuel source in future. Photoelectrochemical (PEC) water splitting using semiconductor materials is a promising means of producing green hydrogen without the generation of carbon dioxide. Semiconductor materials capable of absorbing a wide range of visible light are required to achieve high solar-to-hydrogen (STH) energy conversion efficiency thermodynamically. Perovskite-type oxynitrides AB(O,N)₃ (A=Ca, Sr, Ba and La, B=Ti, Nb and Ta) are potential semiconductors for PEC water splitting in that they are capable of absorbing long wavelengths of visible light and have appropriate band structures spanning water redox potentials. Among the perovskite oxynitrides, BaNbO₂N has an especially small band-gap energy of 1.7 eV ($\lambda < 740$ nm), thus leading to high thermodynamic STH energy conversion efficiency. In this study, we present synthetic conditions of the BaNbO₂N semiconductor and photoanode fabrication using the particulate oxynitride for enhanced PEC activity. The synthesis of small oxynitride particles was investigated for large surface areas of the photoanodes to maximize the light harvesting during the PEC water splitting. To control the particle size of the oxynitride, starting oxides Ba₅Nb₄O₁₅ were prepared by a polymerized complex method and subsequent calcinations at different temperatures of 973, 1073, 1173, and 1273 K. The different Ba₅Nb₄O₁₅ series were nitrated at 1123 K for 13 h to synthesize the corresponding BaNbO₂N. Subsequently, the photoelectrodes made of the different sizes of BaNbO₂N were evaluated for the water splitting under simulated sunlight. Therefore, we will discuss in detail the physical properties of the BaNbO₂N and PEC activity of the photoanodes in a poster presentation.

Poster Presentation : **ELEC.P-778**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Bifunctional Electrocatalyst for Overall Water Splitting at Bimetallic AuRu Alloy Nanofibers in Acidic Environments

Taehui Kwon, Chongmok Lee, Youngmi Lee*

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

Hydrogen has been noted as a non-polluting and practical alternative energy to fossil fuels. Water electrolysis is one of the most important technology to produce hydrogen from abundant renewable sources, however, this reaction is thermodynamically difficult with high overpotentials for OER at anode and HER at cathode. In general, typical HER catalysts with good activity in acidic conditions, such as Pt, exhibit poor activity in OER. Bifunctional electrocatalysts of which activities are good for both OER and HER is beneficial for device simplicity. In this work, we demonstrate the synthesis of AuRu alloy nanofibers (NFs) as bifunctional electrocatalysts for overall water splitting in acidic media. First, Au/RuO₂ nanocomposites are synthesized through electrospinning and calcination, and then AuRu alloy NFs are formed with a subsequent reduction process. The synthesis and morphologies of Au/RuO₂ nanocomposites and AuRu alloy NFs are studied with FE-SEM and TEM. The physical properties of AuRu alloy NFs are analyzed by XRD and XPS and compared to those of pure Au and Ru metal counterparts. The electrocatalytic activity of AuRu alloy NFs are studied toward both OER and HER in acidic solutions with RDE voltammetry. Furthermore, density functional theory (DFT) calculations are conducted to analyze the hydrogen adsorption energy on Ru and AuRu alloy. The performance of AuRu alloy NFs as a bifunctional electrocatalyst for overall water splitting are compared with those of Au/RuO₂, RuO₂, Ru, Pt/C and Ir/C in acidic conditions. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984).

Poster Presentation : ELEC.P-779

Electrochemistry

Zoom 20 FRI 15:00~16:00

Electrospun Iridium-Cobalt Alloy Nanotubes as an Advanced Overall Water Splitting Electrocatalyst at pH-Universal Conditions

Yoonkyeong Kim, Chongmok Lee, Youngmi Lee*

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

Due to lack of fossil fuels, the need for environment-friendly energy system has been emphasized. Hydrogen fuel cell has been considered as the replacement of fossil fuels on account of its extensive advantages such as its large energy capacity. One of the most important ways to produce hydrogen is water splitting, which generally uses precious platinum as a catalyst. Accordingly, the necessity of relatively low-cost catalysts for water-electrolysis has been recognized since large overpotentials are required for both cathodic and anodic reactions of water-electrolysis. Herein, we synthesize iridium-cobalt oxide nanocomposites via electrospinning and calcination process. After thermal treatment with flowing hydrogen gas, bimetallic iridium-cobalt alloy nanotubes are formed. Physical properties are analyzed by FE-SEM, EDS, and TEM. Especially with XRD, the structure of iridium-cobalt alloy is investigated, which comes out to be amorphous structure of face-centered cubic. Electrochemical tests are performed with rotating disk electrode (RDE) voltammetry in 1 M NaOH, 0.5 M H₂SO₄, and 1 M PBS solution to figure out their activities at pH-universal conditions. Overall water splitting tests with two-electrode system are involved to prove of their electrocatalytic activities. Synthesized iridium-cobalt alloy nanotubes exhibit highly effective electrocatalytic behavior in both oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). This bimetallic catalyst - alloy of noble and non-noble metal - shows outstanding activities than Ir/C and Pt/C. This research was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984).

Poster Presentation : ELEC.P-780

Electrochemistry

Zoom 20 FRI 15:00~16:00

Fabrication of a H₂S/Ca²⁺ Dual Electrochemical Microsensor and Its Application to *In Vivo* Monitoring during an Epileptic Seizure in Rat Brain

Jaeyoung Lee, Youngmi Lee*

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

Recent studies show that hydrogen sulfide (H₂S), known to be toxic, plays important roles in various physiological processes as a neurotransmitter. On the other hand, calcium ion (Ca²⁺) is a second messenger in signal transduction, modulating the activation of multiple enzymes. The correlation between H₂S and Ca²⁺ has been investigated in a wide variety of topics in physiology and pathology. In this research, we develop an electrochemical dual microsensor for real-time simultaneous measurement of H₂S and Ca²⁺ and monitor their behaviors during an epileptic seizure in rat brain. A dual sensor is fabricated based on two Pt microwires (50 μm in diameter) embedded in each barrel of a theta-glass capillary. The disk-shaped electrode surfaces are etched and then modified by employing suitable electrochemical techniques. For H₂S detection, Au metal is electrodeposited on one Pt microdisk, followed by electropolymerization of aniline using cyclic voltammetry. For Ca²⁺-selective electrode, Ag metal is electrodeposited on the other Pt disk and oxidized to be coated with a AgCl layer. Ca²⁺-selective membrane is loaded on the electrode, following the surface silanization. Each electrode shows high sensitivity to the target and small selectivity coefficient (below -3) over potential biological interferences. For *in vivo* experiments, we use rat models of seizures induced by 4-AP and measure that H₂S level rises by 1.00±0.04 μM while extracellular Ca²⁺ level decreases by 0.15±0.05 μM during a seizure (n=5). This research was supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984).

Poster Presentation : **ELEC.P-781**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Palladium/Tungsten Oxide Composite Nanofibers for Favorable Oxygen Reduction Reaction.

Seungsun Shin, Chongmok Lee, Youngmi Lee*

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

Proton exchange membrane fuel cells (PEMFCs) have many advantages of low operating temperature, continuous operation at high current density. Oxygen reduction reaction (ORR), a cathodic reaction of PEMFCs, has high overpotential due to multiple electron transfer reaction steps. Therefore, a high-performance electrocatalyst is required for PEMFCs commercialization. Typically, platinum (Pt) is considered one of the most effective catalysts for ORR. However, the practical application of Pt catalyst to PEMFC is demanding due to the high cost, scarcity, and poor stability. Therefore, developing electrocatalysts for ORR regarding both activity and stability at a low cost remains a significant challenge. In this study, we synthesized Pd/WO_{3-x} composite nanofibers (NFs) and then measured electrocatalytic activity and stability of this material for ORR in 0.1 M NaOH aqueous solution. First, PdO/WO₃ was synthesized by electrospinning and subsequent calcination. After the thermal treatment of PdO/WO₃ under H₂ atmosphere, Pd/WO_{3-x} composite NFs were formed. The morphologies and composition of the synthesized catalysts were characterized by SEM, EDS, XRD and XPS. Electrochemical experiments were conducted using rotating disk electrode (RDE) voltammetry. We also measured the electrocatalytic performance of Pd NFs, Pt/C, and Pd/C toward ORR for comparison. The overall performance of Pd/WO_{3-x} NFs exhibits favorable ORR activity and remarkable stability over other samples. Herein, Pd/WO_{3-x} NFs are qualified as promising electrode materials for ORR. This research was supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT& Future Planning (NRF-2020R1A2B5B01001984).

Poster Presentation : **ELEC.P-782**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Size Effect of Redox Molecules on Nanoporous Platinum: Alcohol Electrooxidation

Je Hyun Bae^{*}, Taek Dong Chung^{1,*}

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

¹Department of Chemistry, Seoul National University, Korea

Nanoporous electrodes have been attracting much attention for diverse applications such as energy conversion devices and sensors. Electrochemical features of nanoporous electrode arising from their morphology markedly distinct from those of flat electrode. We examined this morphological effect on electrochemical reaction through a widely renowned electrochemical reaction, alcohol electrooxidation, which is closely related to many electrochemical devices including fuel cell. In this work, the electrocatalytic behavior of nanoporous Pt was investigated by cyclic voltammetry and electrochemical impedance spectroscopy. And, molecular size effect was probed to unravel the origin of electrocatalytic potential of nanoporous electrodes.

Poster Presentation : **ELEC.P-783**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Bimetallic ZIF-derived CoNi nanostructures for efficient reversible oxygen electrocatalysis

Sunguk Noh, Jun Ho Shim*

Department of Chemistry, Daegu University, Korea

Oxygen electrocatalysis, oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), governs the performance of various electrochemical energy systems such as metal-air batteries, fuel cells, and water electrolyzers. However, the slow rates of these two reactions and their dependency on expensive precious metal nanocatalysts prohibit the sustainable commercialization of these technologies. On the other hand, metal organic framework (MOF) catalysts are identified as multi-dimensional porous polymeric crystalline organic-inorganic hybrid materials with outstanding properties including a high specific surface area, huge pore space, and ordered crystalline structure. MOF-based catalysts often exhibit higher catalytic activity than their corresponding homogenous catalysts as demonstrated in many catalytic reactions. Zeolitic imidazolate framework (ZIF) is one of the subclasses of MOFs with a similar structure to zeolites. It has attractive structural properties and intrinsically lower density. In this study, the CoNi nanostructures were synthesized by a two-step reaction of carbonization with ZIF followed by corrosion. Composition and structural features were characterized by a scanning electron microscope equipped with an energy dispersive X-ray spectroscopy, high-resolution transmission electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy. Electrocatalytic activity for both ORR and OER in alkaline medium was investigated by rotating disk electrodes and rotating ring disk electrodes and cyclic voltammetry. Indeed, it was confirmed that ORR/OER activity increased through carbonization and corrosion process. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614).

Poster Presentation : **ELEC.P-784**

Electrochemistry

Zoom 20 FRI 15:00~16:00

In-situ Spectroelectrochemical Analysis of CsPbX₃ for Tracking their Transformation

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All-inorganic lead halide perovskite quantum dots (CsPbX₃, X: Cl, Br, or I, abbreviated as PQDs) operate successfully in various optoelectronic devices, such as solar cells, LEDs, photocatalysis, lasing, and so on. These devices work under electrochemical bias and/or illumination with charge separation/collection by interacting with charge transport medium. To investigate photoinduced charge transport or charge injection via applied bias using electrochemical and photochemical tools, it is essential to consider not only each but also simultaneous. In-situ spectroelectrochemical method provides quantitative insights about the spectroelectrochemical behaviors of the CsPbBr₃ and CsPbI₃ PQDs. Also, we found that these PQDs underwent irreversible transformation to precursor state of plumbate complexes under electrochemical conditions. Beyond the certain applied bias, we were able to monitor that hole mediate electrochemical oxidation of the PQD impacts the irreversible transformation. By Understanding such charge transfer mediated process, we could know the way to develop practical strategy for utilization of the PQDs to optoelectronic devices.

Poster Presentation : **ELEC.P-785**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Bimetallic Fe-Co/Fe-Ni nanocomposites enabling highly efficient electrochemical water oxidation

Yun Hwi Seong, Yongdeog Kweon, Jun Ho Shim*

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Water electrolysis to generate oxygen and hydrogen has been a major focus of electrochemical energy conversion and storage research. However, this field still faces challenges of large overpotential, slow electron transfer kinetics, and limiting commercial viability, despite advances achieved in the electrocatalytic oxygen evolution reaction (OER). In this presentation, we describe the latest advances in electrocatalytic water oxidation using bimetallic Fe-Co and Fe-Ni materials. The electrocatalytic activity of the transition bimetals for OER in alkaline media was investigated by rotating disk electrode, rotating-ring disk electrode, and cyclic voltammetry. The high catalytic performance was ascribed to the porous structure, which provided more active sites and was beneficial to a high-flux mass transportation. The prepared Fe-Co or Fe-Ni catalysts were characterized by field emission scanning electron microscopy, high-resolution transmission electron microscopy, X-ray diffraction, X-ray photoelectron spectroscopy to examine the structural features. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614).

Poster Presentation : ELEC.P-786

Electrochemistry

Zoom 20 FRI 15:00~16:00

Preparation of TEMPOL and Oxo-TEMPO Derivatives : Tempol and Oxo-tempo Adsorbed Li-TFSI Film for Fiber-Shaped Dye-Sensitized Solar Cell.

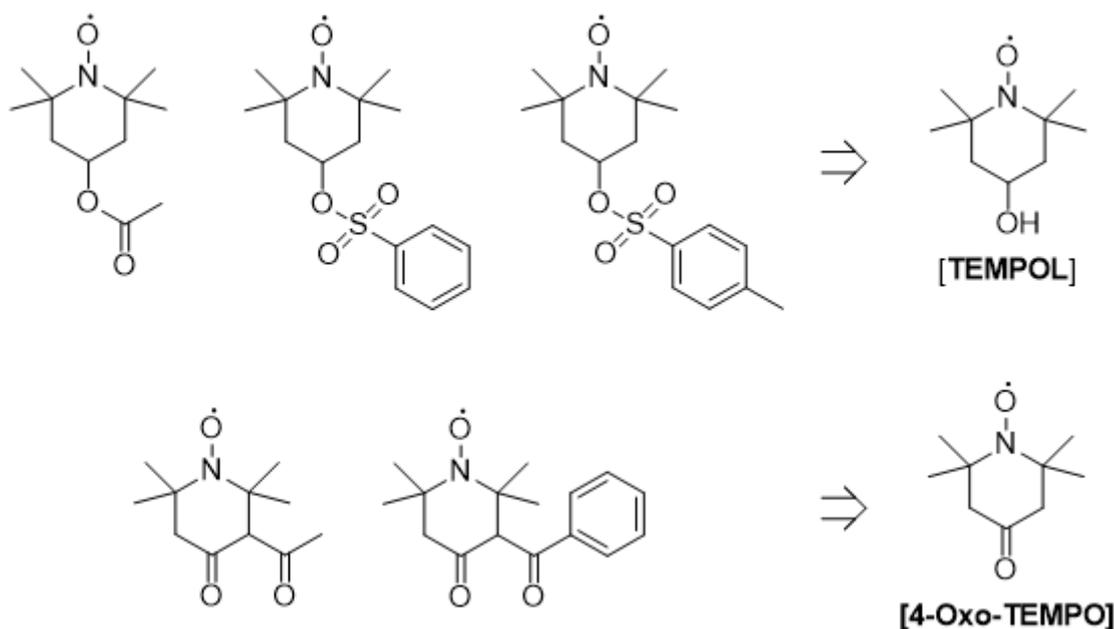
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Fiber-shaped solar cells (FSCs) have attracted academically and industrially intense interest due to their light weight, flexibility, weavability, and wearability. FS-DSSC using Li-TFSI film as a quasi-solid-state electrolyte with both traditional electrolyte and TEMPOL and Oxo-TEMPO electrolyte were first designed. The TEMPOL and Oxo-TEMPO derivatives as electrolyte were prepared conveniently.



Poster Presentation : ELEC.P-787

Electrochemistry

Zoom 20 FRI 15:00~16:00

As a Solid State Electrolyte(SSE) for All Solid State Battery, Improved Electrochemical stability of Oxygen-Doped Argyrodite $\text{Li}_{5.5}\text{PS}_{4.5}\text{Cl}_{1.5}$ with Ionic Conductivity of ~ 3.3 mS/cm

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In the near future, the demand for electric vehicles is expected to increase more rapidly than for internal combustion engine vehicles, and the demand for more stable batteries is expected to increase. According to these changes, various battery-related companies are trying to maximize the stability of batteries so that many users can be safe from explosion and fire. Due to these efforts, the need for an all-solid-state battery is currently emerging. For this reason, the development of solid-state-electrolyte materials is essential. Among many solid state electrolytes, $\text{Li}_6\text{PS}_5\text{Cl}$, which has high ionic conductivity, shows the ionic conductivity of about 2 mS/cm. However, the ionic conductivity of $\text{Li}_6\text{PS}_5\text{Cl}$ is significantly lower than that of other liquid electrolytes, and is not sufficient for commercialization due to poor interfacial stability and air stability. To solve these problems, we synthesized $\text{Li}_{5.5}\text{PS}_{4.5}\text{Cl}_{1.5}$ with ionic conductivity of 4.8 mS/cm. And then, some sulfur was replaced by oxygen to improve interfacial stability, air stability and ultimately electrochemical stability. The oxygen-doped $\text{Li}_{5.5}\text{PS}_{4.0}\text{O}_{0.5}\text{Cl}_{1.5}$ and $\text{Li}_{5.5}\text{PS}_{3.5}\text{O}_{1.0}\text{Cl}_{1.5}$ were decreased the conductivity to 4.3 mS/cm and 3.3 mS/cm. However, in the Galvanostatic cycle test, the two samples showed more stable voltage profiles than the conventional $\text{Li}_{5.5}\text{PS}_{4.5}\text{Cl}_{1.5}$ and significant improvement in air stability in the XRD pattern over time of exposure to air. These results can also be expected to inhibit Li-dendrite in the interface when a full-cell or half-cell is assembled using oxygen-doped argyrodite. So these results confirm the possibility of argyrodite becoming a more stable material as a solid state electrolyte and showing improved electrochemical performance in the future.

Poster Presentation : **ELEC.P-788**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Ultra-low Ru loading nanocatalyst for hydrogen evolution and oxygen reduction reactions

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The low cost renewable energy, such as hydrogen-involving energy conversion reactions, to replace fossil fuels has been studied for a long time, but fundamental and practical challenges remain. In water electrolysis, H₂ generation at the cathode through the hydrogen evolution reaction (HER), essentially developed as a Pt catalyst. However, platinum catalysts are expensive and thus there have been numerous efforts to minimize the use of Pt in the catalyst layer by increasing activity. On the other hand, ruthenium-based materials for HER are very promising because of their prominent catalytic activity and the cheapest price among the precious metal family. Herein, an ultra-low Ru loading nanocatalyst was synthesized by a convenient aqueous chemical growth on Pd-nanochain networks (denoted as Ru-on-nPd/C). A significant enhancement in electrocatalytic HER properties has been achieved by decorating a trace amount of Ru clusters on the surface of Pd nanochain. This material was also investigated as ORR catalysts. The compositional/structural features were characterized by high-resolution transmission electron microscopy, X-ray photoelectron spectroscopy and X-ray diffraction. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1F1A1049614).

Poster Presentation : **ELEC.P-789**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Synthesis of WO₃ microplate electrode for ultrasensitive acetone detection

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Recently breath analysis has attracted a lot of attention for monitoring health and early diagnosis of diseases. Typically, acetone is investigated as a biomarker in the exhaled breath of diabetic patients. Many metal oxides have been intensively studied as semiconducting sensors to detect acetone. However, it is still difficult to selectively and accurately analyze trace acetone gas in the exhaled breath. Here in, we successfully synthesized tungsten oxides (WO₃) microplates for the fabrication of gas sensor device. Solvothermal method was employed to synthesize pristine WO₃ microplates. The WO₃ microplate-based chemiresistive sensors exhibited a rapid response, superior sensitivity, and highly selective detection of an acetone gas. Typically, the WO₃ microplates exhibited an ultrasensitive response to acetone gas, with a response up to 8.12 (R_a/R_g) toward 1 ppm acetone at 400 °C. This represents a higher response compared to other WO₃ materials. The influence of the crystal structure of WO₃ and the nature of the surface facets were fully investigated. This study highlights the possibility of the rapid detection toward acetone for the development of advanced chemical sensors.

Poster Presentation : **ELEC.P-790**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Highly Efficient and stable g-C₃N₄ decorated Ta₃N₅ Nanotube for Photoelectrochemical Water splitting

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Tantalum nitride (Ta₃N₅) nanotubes (NTs) is an up-and-coming visible-light-driven photoelectrode for photoelectrochemical (PEC) water splitting with a narrow band gap of approximately 2.0 eV that can utilize a large fraction of the solar spectrum up to 600 nm to enhance the photocatalytic activities. Herein, we were deposited Ta metal film onto the n-Si wafer substrate by magnetron sputtering technique and developed a Ta₃N₅ NTs thin-film photoanode with a length of approximately ~1.3 μm by an electrochemical anodization in a fluorinated-based electrolyte. Results showed that the film annealed at 700°C for 7h exhibited high crystallinity, high visible light absorption, and a highly conductive interlayer between the substrate, resulting in the highest photocurrent density (JSC) of ~0.26 mA/cm² at 1.23 VRHE in PEC water splitting. Although, this photoelectrode is suffered from its special self-oxidation problem under photoelectrochemical (PEC) water splitting conditions. Based on this electrode, to enhance the photostability and PEC performance of Ta₃N₅ NTs, g-C₃N₄ thin layer with an energy band gap of about 2.7 eV was deposited by an electrophoretic method under constant potential (20 V) for 30 sec, 1, 2, 3 and 4 min respectively because of its several unique identical key properties such as thermal stability, robust fabrication process, reasonable band alignment, and it responds to absorb visible light. With increasing the deposition time of the g-C₃N₄ layer to 2 min, the g-C₃N₄ thin layer steadily covered the surface area of Ta₃N₅ NTs and exhibited the highest photocurrent density (JSC) of ~0.59 mA/cm² at 1.23 VRHE under the solar light irradiation. The modified g-C₃N₄/Ta₃N₅/Si photoelectrode showed an excellent photostability and photocatalytic PEC performance.

Poster Presentation : **ELEC.P-791**

Electrochemistry

Zoom 20 FRI 15:00~16:00

Charge Transfer Complex Cu-TCNQ Integrated TiO₂ Nanotubes for Efficient Solar Water Splitting

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The increasing energy demand and environmental pollution are today's most important problems and the scientific community is searching a new form of energy alternative to fossil fuels which is one of the primary research topics of the 21st century. Hydrogen is the fuel of the future because of high gravimetric energy density and clean combustion. Hydrogen can be produced by photoelectrochemical water splitting method by using semiconductor photoanode/photocathode. The efficient, stable, visible light absorption and cost effective photoelectrode materials are certainly important in developing highly efficient PEC system. TiO₂ is the most widely investigated photocatalyst for PEC water splitting due to their low cost, non-toxicity, high chemical and thermal stability. In the present work, we have integrated the charge transfer complex Cu-TCNQ (Copper-Tetracyanoquinodimethane) with TiO₂ nanotubes (NTs) for PEC water splitting application. The Cu-TCNQ nanocrystals (NCs) were incorporated onto the surface of TiO₂ NTs by electrophoretic method. The fabricated Cu-TCNQ/TiO₂ NTs heterojunction photoanode was systematically characterized by using various techniques. Owing to the good electrocatalytic activity of Cu-TCNQ co-catalyst, the Cu-TCNQ/TiO₂ NTs heterojunction photoanode exhibited remarkably enhanced photocurrent density when compared to bare TiO₂ NTs. The significant enhanced PEC performance is mainly due to the integrated Cu-TCNQ co-catalyst on the surface of TiO₂ NTs, which greatly minimizes the possibility of electron-hole pair recombination.

Poster Presentation : ELEC.P-792

Electrochemistry

Zoom 20 FRI 16:00~17:00

Synthesis of PANI@ α -NT (PANI@ α -Fe₂O₃) Nanocomposite as Advanced Electrode Materials for Supercapacitor Applications

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In this work, we report a facile synthesis of one-dimensional α -Fe₂O₃ hollow nanotubes using anodic aluminum oxide (AAO) template-assisted materials and PANI decorated α -Fe₂O₃ hollow nanotubes (NTs) as PANI@ α -Fe₂O₃ hollow nanotubes for supercapacitor applications. The thickness of the nanotubes enhanced significantly on increasing growth time. Hence, synthesized at 3 hours of α -Fe₂O₃ hollow NTs as a materials display an internal diameter of 50-100 nm with external diameter of 150-250 nm as evidenced by SEM and TEM microscopic images. Furthermore, PANI decorated α -Fe₂O₃ hollow nanotubes (PANI@ α -Fe₂O₃ NTs) contain organic conducting-polymer, polyaniline (PANI) which showed low-conductivity and low capacitance. Interestingly, PANI@ α -Fe₂O₃ NTs achieved significantly improved capacitance compared to reference α -Fe₂O₃ hollow NTs due to PANI incorporation in α -Fe₂O₃ hollow NTs which modified its structure. To improve the electrochemical performance, α -Fe₂O₃ hollow NTs were combined into the hollow nanotube and outside of nanotube with PANI to obtain PANI@ α -Fe₂O₃ hollow NT-a as a specifically named after (PANI@ α -NT-a) and α -Fe₂O₃ hollow NTs were combined only into the hollow nanotube with PANI to obtain PANI@ α -Fe₂O₃ hollow NT-b as a specifically named after (PANI@ α -NT-b). The PANI@ α -NT-a electrodes with specific capacitance of 186.6Fg⁻¹ and 63.5Fg⁻¹ at a current density of 0.5Ag⁻¹ respectively. The PANI@ α -NT-a electrodes have exhibited good cycling stability of 90.58% after 1000 cycles with a scan rate of 10mV-1. The results of PANI@ α -NT-a electrodes have excellent potential as supercapacitor applications as high-performance energy storage devices in future.

Poster Presentation : **ELEC.P-793**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Shape-controlled Palladium Hydride Nanocatalysts toward Oxygen Reduction Reaction

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Oxygen reduction reaction (ORR) commencing at the cathode of proton exchange membrane fuel cells (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 recognized as the most active toward the ORR, palladium (Pd) has also drawn substantial attention as potential electrocatalysts in acidic and alkaline media. This presentation reports Pd octahedra and cubes enclosed by {111} and {100} facets, respectively, and their hydride forms (PdH), which were prepared to probe the shape and composition effects on ORR. The hydriding effect improved the ORR performance on the PdH octahedra compared with Pd octahedra. Conversely, PdH cubes showed a decrement in ORR activity compared to Pd cubes. The opposite trend of the hydriding effect in relation to shape was supported by Sabatier's principle, where the optimal OH binding strength of nanocatalyst governs ORR activity. Reference[1] M. K. Kabiraz, J. Kim, S.-I. Choi, Bull. Korean Chem. Soc. 2021.[2] M. K. Kabiraz, J. Kim, W.-J. Lee, B. Ruqia, H. C. Kim, S.-U. Lee, J.-R. Kim, S.-M. Paek, J. W. Hong, S.-I. Choi, Chem. Mater. 2019, 31, 5663.[3] M. Shao, T. Yu, J. H. Odell, M. Jin, Y. Xia, Chem. Commun. 2011, 47, 6566.

Poster Presentation : **ELEC.P-794**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Electrochemical deposition of carbon-based nanocomposite for amperometric dopamine sensor

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Cogno-Mechatronics Engineering, Pusan National University, Korea

A simple electrochemical synthesis of carbon-based nanomaterials is highly desirable for non-enzymatic electrochemical sensors these days. In this work, we describe a one-step electrochemical deposition technique to prepare electrochemically reduced graphene oxide (ErGO), multi-walled carbon nanotubes (MWCNTs), and polypyrrole (PPy) nanocomposite (ErGO/MWCNTs/PPy) in neutral solution for dopamine (DA) detection. The prepared sensor shows improved electrocatalytic performance towards DA that can be contributed to the π - π^* stacking interactions between ErGO, MWCNT and PPy. The physical and electrochemical properties of the nanocomposites could be evaluated through field emission scanning electron microscopy, Raman spectroscopy, electrochemical impedance spectroscopy, cyclic voltammetry and chronoamperometry. The sensor was optimized by means of applied potential, pH of the solution and temperature and details will be presented in the poster. The sensor sensitivity was calculated to be $8.96 \mu\text{A mM}^{-1} \text{cm}^{-2}$, and the wide linear range was from 25 nM to 1000 nM ($R^2 = 0.999$). The limit of detection of the sensor was 2.3 nM with no distinct interferences observed for other electroactive species.

Poster Presentation : **ELEC.P-795**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Electrochemistry of Pickering emulsions

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Pickering emulsions are valuable in various fields such as drug delivery, pharmaceutical, cosmetics, and food industry, due to advantages such as excellent stability and biocompatibility compared to classical emulsions. In this study, we first revealed the possibility of electrochemical reactions of Pickering emulsions, and their applications in electrochemical nanomaterial synthesis. Stable water-in-oil (w/o) Pickering emulsions of submicron size were formed solely with hydrophobic silica nanoparticles as capping agents. The emulsions were characterized by dynamic light scattering, optical microscopy, and confocal laser scanning microscopy. The electrochemical reaction caused by the single Pickering emulsion droplet landing on the working electrode was observed in situ by electrochemistry and inverted fluorescence microscopy. Ag⁺ ions confined in the Pickering emulsions were reduced to synthesize surfactant-free silver nanoparticles on the electrodes. We will apply Pickering emulsions as a metal nanoparticle synthesis medium to control size, composition, and spatial distribution.

Poster Presentation : **ELEC.P-796**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Electrodeposition of graphitic carbon nitride on the glassy carbon electrode for selective detection of 5-hydroxytryptamine

Thenmozhi Rajarathinam, Miri Yeom, Seung-Cheol Chang*

Cogno-Mechatronics Engineering, Pusan National University, Korea

An easy one-step electrodeposition of graphitic carbon nitride ($g-C_3N_4$) is inevitable for non-enzymatic sensor designs. In this report, we constructed a sensor based on the electrochemical approach that readily exfoliates the bulk $g-C_3N_4$ to two-dimensional $g-C_3N_4$ nanosheets. The exfoliation was carried out at optimized potential +1.75 V for 100 s under neutral pH conditions. Physical and electrochemical characterizations were carried out to evaluate the sensor performance. The optimized sensor serves as an electro catalyst for highly sensitive and selective amperometric detection of 5-hydroxytryptamine (5-HT) or serotonin. The $g-C_3N_4$ nanosheets sensor demonstrates a wide linear range from 500 pM to 1000 nM ($R^2 = 0.999$). The limit of detection and sensitivity of the fabricated sensor was calculated to be 150 pM and $1.03 \mu A \mu M^{-1} cm^{-2}$, respectively. The two-dimensional $g-C_3N_4$ nanosheets sensor platforms open new avenues for 5-HT detection at the ultra-low concentration ranges. The experimental parameters such as applied potential, pH, selectivity, reproducibility and storage stability were optimized and will be presented in the poster.

Poster Presentation : **ELEC.P-797**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Lithium air battery cathode analysis with Scanning Electrochemical Microscopy

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Because of high specific energy density of lithium air battery, many studies have been conducted on lithium air batteries towards electrical vehicles (EV) application. However, low cyclability of cathode interferes long term operation of lithium air battery. In particular, researchers have focused on understanding the electrochemistry of chemical species upon discharge at cathodes, particularly lithium peroxide (Li_2O_2), to resolve the cyclability issue. In this regard, we employed scanning electrochemical microscopy (SECM), in-situ electrochemical probe imaging instrument, to analyze the electrochemical property of lithium peroxide with nanometer spatial resolution. Electron transfer and hydrolysis rates of two types of Li_2O_2 will be evaluated in this presentation.

Poster Presentation : **ELEC.P-798**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Bulk and surface Fe coupled OER activity boosting of Ni_{1-x}Fe_xOOH Nanosheets

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Fe-based electrocatalysts, especially with Ni is attractive for oxygen evolution reaction (OER) in alkaline environment due to their exhilarating surface properties and anticipated synergistic effect. However, the effects of Fe on the catalytic performance and sustainability with regard to its position in the main catalyst part have not yet fully understood. Here, we report an investigation of systematically incorporated bulk Fe (FeB) or surface Fe (FeS) and their synergistic effect on the electrochemical behavior and OER activities of a series of Ni_{1-x}Fe_xOOH (x: 0, 0.25, 0.50, 0.75, and 1) nanosheets (NSTs) to provide new insight into their activities. Different ratios of Fe and Ni precursor was deposited on nickel foam (NF) cathodically for FeB embodiment. Then, surface Fe is integrated through anodic cycling from Fe-containing KOH. The result shows that both bulk and surface Fe are essential to achieve higher OER activity and stability. Accordingly, both bulk and surface Fe incorporated NST at x = 0.25, i.e., FeB+S-NiFe_{0.25} has demonstrated the highest OER activity, with lowest overpotential of 200 mV at a current density of 10 mA cm⁻², a Tafel slope as low as 30 mV dec⁻¹, and robust stability exceeding 100 h for continuous oxygen generation while the same NST in the absence of surface Fe, has demonstrated a higher overpotential of 260 mV and a Tafel slope of 65 mV dec⁻¹. It is probable that the cooperation of bulk and surface Fe induces high OER activity and can be readily applied to generate cheap and clear energy. Keywords: Bulk and surface Fe, electrocatalyst, NiFe oxyhydroxide nanosheets, oxygen evolution reaction, synergistic effect

Poster Presentation : **ELEC.P-799**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Plasma assisted exfoliation of NiFeCo LDH nanosheets for enhanced OER

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Hydrogen energy with high mass energy density and renewability is widely recognized to be an alternative fuel for the near future. Hydrogen gas can be produced from different sources by different methods. For instance, water splitting into hydrogen and oxygen by electrolysis using electricity from renewables is one of the easiest and cleanest methods for high-purity hydrogen production and an effective way to store the excess electrical power. However, oxygen evolution reaction is usually considered as a limiting rate reaction for electrocatalytic water splitting because it is a one-step, four electron reaction with sluggish kinetics and high overpotential. To date, noble metal based electrocatalysts have demonstrated favorable OER activity. But their high cost and insufficient stability severely prohibit their further largescale industrial applications. Thus, exploring highly efficient electrocatalysts for oxygen evolution reaction is imperative. First row transition metal compounds have been regarded as an attractive family of inexpensive and highly efficient electrocatalysts toward water splitting. However, their electrocatalytic activities are significantly limited by their low electrical conductivity and stability. Recently, different techniques have been employed to improve the electrocatalytic activities of the transition metal compounds. Among the techniques, plasma treatment has emerged as a powerful approach to increase the exposure of the active edge sites so as to improve the surface utilization and catalytic activity. Herein, we studied the electrocatalytic effects of O₂-plasma treated NiFeCoO_x nanosheet electrochemically deposited on NF nickel foam. Benefiting from the large electrochemical surface area and exposed active sites, the catalyst has exhibited extraordinary water oxidation performance in alkaline media.

Poster Presentation : **ELEC.P-800**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Improving Activity of Metal Alloy Nanoparticles for Hydrogen Evolution Reaction by Creating Surface Defects

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Rational designs of electrocatalysts, including increased catalytic surface area, unique surface structure, and enhanced the conductivity, have been developed to improve the hydrogen evolution reaction (HER). In this work, defect engineering on catalyst surfaces of FeMe nanoparticles is considered an effective and feasible way to accelerate the HER kinetics. By etching the surface Fe atoms using HF treatment, a defect-rich surface of FeMe alloy nanoparticles was prepared. Surface atomic defects on FeMe nanoparticles were successfully analyzed by X-ray absorption spectroscopy, high-resolution photoemission spectroscopy, and electrochemical absorption/desorption experiments. The defect-rich FeMe-based nanocatalyst exhibited 14 and 19 mV overpotential reduction compared to the state-of-the-art Ru/C and Pt/C catalysts, respectively.

Poster Presentation : **ELEC.P-801**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Preparation of the nitrogen and another hetero-atom co-doped carbon-based non-precious metal catalyst toward the oxygen reduction reaction

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The Pt-based catalysts have shown remarkable oxygen reduction reaction (ORR) catalytic performance so far. Because of the high prices and low stability of Pt-based catalysts, non-precious metal catalyst (NPMC) was studied by many researchers to alternate Pt-based ORR catalysts. The hetero-atom doped carbon material has a variety of properties depend on doped hetero atoms. For this reason, hetero-atom doped carbon materials are used in various ways. The nitrogen-doped carbon materials are well known for their advantages in ORR activity. In this work, we prepared NPMC with the iron atoms chelated by an ethylenediamine (EDA) and another hetero-atom (sulfur or fluorine) added to make a synergistic effect with nitrogen atoms toward ORR performance. The prepared catalysts were compared ORR activity with the Fe@CN which was doped nitrogen and iron atoms on the carbon material. The ORR catalytic performance of the catalysts was measured in acidic and alkaline media. The Fe@CN-S co-doped as nitrogen and sulfur increased nitrogen contents on the surface of the catalyst. Furthermore, the ratio of pyridinic N and graphitic N which have an advantage of ORR was increased. Fe@CN-F co-doped as nitrogen and fluorine showed the same onset potential as Fe@CN-S in the acidic media. Fe@CN-F showed higher onset potential than Fe@CN-S in the alkaline media. Fe@CN-F showed good ORR performance, despite Fe@CN-F was not increased the amount of nitrogen atom. The C-F bonds in the Fe@CN-F may occur as a new active site.

Poster Presentation : **ELEC.P-802**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Synthesis of hollow-structured tantalum oxide as electrochemical catalyst support for oxygen reduction reaction and Pt/H-Ta₂O₅ catalyst performance evaluation

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To improve oxygen reduction reaction (ORR) activity and stability of the cathodic catalysts in PEMFCs, increasing the durability of the catalyst support is an important part. Many researchers have developed various materials for the durability of the catalyst supports, such as carbon nanotubes, mesoporous carbon, carbon nanofibers, and metal oxides. In this work, hollow tantalum oxide (H-Ta₂O₅) was synthesized as electrocatalyst support for ORR. Ta₂O₅ has high mechanical strength and durability, so it can be used as electrocatalyst support. The H-Ta₂O₅ was obtained after removing the silica nanospheres through NaOH etching. The structure of H-Ta₂O₅ was characterized by SEM and TEM. N₂ adsorption/desorption analysis was performed to obtain the BET specific surface area and BJH pore size of H-Ta₂O₅. Pt/H-Ta₂O₅ was synthesized by impregnating H-Ta₂O₅ with Pt in an appropriate amount, and the ORR performance of Pt/H-Ta₂O₅ was compared with commercial Pt/C.

Poster Presentation : **ELEC.P-803**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Evaluation of the effective capacitance and resistance of a constant phase element

Byoung-Yong Chang

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In analysis of electrochemical impedance spectroscopy, constant phase elements (CPE) are usually used as capacitive elements. Therefore, the effective capacitance of the constant phase element can be estimated by converting the constant phase element to its equivalent capacitor. Electrochemical impedance spectroscopy can resolve a complex electrochemical process into its faradaic and non-faradaic processes. Over the analysis processes, the non-faradaic process is frequently described as a CPE in place of a capacitor because an aqueous system cannot have a solid electric double layer. When it is represented as a capacitor, the non-faradaic element finds the information by means of the capacitance, but when represented as a CPE, the information is hardly evaluated simply through the capacitance. In order to solve the problem, the CPE is dealt with as an equivalent capacitor of which the capacitance provides practical information. Two similar methods to solve the same problem have been previously reported, but an advanced method is described in this presentation. As the previous methods consider only the CPE for conversion to its equivalent capacitor, the new method applies the correlation between the CPE and its related resistor for the conversion process. We also compare the results obtained by the three methods, and realize that the results are nearly the same within acceptable ranges. Finally, we make a conclusion that any of the methods can be used within acceptable tolerance and that the choice is only dependent on the conditions of the system of interest.

Poster Presentation : **ELEC.P-804**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Entropymetry of the Active Materials for Li-ion Batteries by Temperature Scanning

Byung Yeon Kang, Hyun Deog Yoo^{1,*}

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Abstract It is essential to understand the thermodynamic properties of active materials to determine the batteries performance and the safety. The open circuit voltage (OCV) of an electrochemical cell is a direct measure of the Gibbs free energy as a function of the state of charge (SoC). In this regard, measuring the OCV under the temperature scanning renders the change of entropy and enthalpy, and this technique has been named as entropymetry. The entropymetry is a non-destructive tool to study the thermal properties of lithium-ion batteries (LIBs). Herein, we conduct the entropymetry of the following active materials for LIBs: LiCoO_2 , $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$, LiMn_2O_4 , $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_2$, LiFePO_4 , $\text{Li}_4\text{Ti}_5\text{O}_{12}$, and graphite. Coin-type cells were placed in the temperature-scanning chamber, and the OCV was recorded as a function of the temperature at the SoC of 100% and 50%. Overall, the entropy change of LiCoO_2 and $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ was the largest and the smallest among the cathodes, respectively. This may suggest that the high-nickel cathodes can be more efficient energetically, because the entropy change is related with the waste heat during the electrochemical process. All the active materials exhibited more reversible behaviors at 50% SoC compared to at 100% SoC, due to the side reactions at the higher voltage. This presentation will discuss the thermo-electrochemical properties of other active materials also.

Poster Presentation : **ELEC.P-805**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Effects of Governing Equations on the Computational Speed and Accuracy for the Electrochemical Modeling of Lithium-Ion Batteries

Sang Hyeok Kim, Hyun Deog Yoo*

Department of Chemistry, Pusan National University, Korea

Secondary/rechargeable batteries have turned out to be an indispensable part of our everyday lives. The applications include portable electronics, electric vehicles (EVs), and energy storage systems (ESS). In this context, lithium-ion batteries (LIBs) are significant because of their light-weight and the high energy density. However, the safety and range issues still remain in the larger-scale LIBs. Electrochemical modeling leads to a complete understanding of the physico-chemical behavior of LIBs, which provides guidelines for further development. It is important to raise the level of accuracy and the computational speed for more efficient modeling and management of batteries. The electrochemical modeling is based on governing equations that describe mass transport and charge transfer. There can be different frameworks that produce different governing equations: (i) conservation of mass and charge vs conservation of energy, (ii) descriptors of molar concentration and current density vs intercalation quantity and C-rate, and (iii) descriptors with vs without dimensions. And the above three combinations lead to total eight different sets of governing equations. In this work, an electrochemical model based on the above eight different sets of governing equations were compared in terms of the computational speed and accuracy. The detailed results and discussion will be shared in the presentation.

Poster Presentation : **ELEC.P-806**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Electrochemical deposition of Pd²⁺ emulsion droplets on a C-UME surface

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The development of single-entity electrochemistry (SEE) has led to a very recent application of synthesizing metal nanoparticles which is also called nanodroplet-mediated electrodeposition^{1,2,3}. This research is to synthesize Pd nanoparticles applying the novel method for the first time. Pd is well known as a good hydrogen storage material as well as an active catalyst for direct formic acid fuel cell^{4,5}. We used water-in-oil emulsion droplets containing Pd²⁺ precursor as reactors to electrodeposit on a working UME biased at a suitable constant potential. The synthesized amount of the produced Pd nanoparticles could be managed, and the catalytic activity of the formed nanoparticles for HCOOH oxidation was investigated for broader understanding the properties at nanoscale of the Pd metal. The recent synthetic method promises a simple, fast, effective and non-expensive way could be applied for other catalytic nanoparticles.

Poster Presentation : **ELEC.P-807**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Serotonin in Human Platelets Analyzed by Single Particle Collision Method Based on Single-Entity Electrochemistry

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This study aims to investigate human platelet concentration using serotonin oxidation based on single particle collision method using single-entity electrochemistry (SEE). These experiments can be performed by placing an ultramicroelectrode (UME) in a solution containing platelets to be detected by chronoamperometry. Studies of biomolecule detection using the SEE method could be useful for directly measuring platelet counts based on the fact that serotonin in the blood is stored and transported in platelet granules. Observing current changes due to oxidation of serotonin when platelets collide with UME can provide useful information about platelets or serotonin-related diseases. It is expected that this study will help in early diagnosis of various platelet/serotonin related diseases.

Poster Presentation : **ELEC.P-808**

Electrochemistry

Zoom 20 FRI 16:00~17:00

The Synthesis and characterization of various ratio with hydrophilic polymer-osmium complex and its application for a glucose sensor using glucose dehydrogenase (GDH)

Ryang Hyeon Kim, Yun Yeong Cho, Hyug-Han Kim^{1,*}

Dankook University, Korea

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In this study, we synthesized $\text{Os}(\text{dmo-bpy})_2\text{Cl}_2$ by coordinating 4,4'-dimethoxy-2,2'-bipyridine(dmo-bpy) ligand with the 8th group metal element, osmium, in redox complex, which is an electron transfer. The acrylamide and vinylpyridine were used to synthesize the new hydrophilic polymer, poly(acrylamide)-poly(vinylpyridine)(PAA-PVP), which is a good electrode for the osmium complex and facilitates the electron transfer between enzymes and electrodes. In this study, the hydrophilic polymers were synthesized by the changing ratio of acrylamide and vinylpyridine to confirm the ping-pong mechanism of osmium complex amount. For structural analysis, ¹H-NMR, FT-IR, UV-VIS, XPS and CV were carried out. The CV, multi-potential step and zeta potential were used for checking electrochemical properties. Finally, it was confirmed that high selectivity and sensitivity and catalytic current were generated through reaction between glucose and glucose dehydrogenase (GDH) using electrodes with osmium complex immobilized. Our mediator showed the possibility for applying to the glucose sensor.

Poster Presentation : **ELEC.P-809**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Thermally Induced hcp-Co_xRh_{1-x} Bimetallic Alloy as a pH-independent Catalyst for Hydrogen Evolution Reaction

Dasol Jin, Youngmi Lee^{*}, Myung Hwa Kim^{*}, Chongmok Lee^{*}

Department of Chemistry & Nanoscience, Ewha Womans University, Korea

Considering the increasing interest in electrochemical water splitting, synthesis advanced materials for electrocatalytic water splitting are central to the area of renewable energy. The heterogeneous catalysts such as alloys and composites have long been a subject of study, and the one for HER requires to balance the strengths between the adsorption/desorption of hydrogen on the catalyst surfaces for optimized HER activity. Here we present the physical/electrochemical characterization of single-phase CoRh₂O₄ and their reduced form, Co_xRh_{1-x} nanofibers. And this work introduces a facile synthetic process for the formation of two distinct crystalline phases (i.e., hcp and fcc) of Co-Rh bimetallic alloy nanofibers by thermally treating the single phase CoRh₂O₄ under H₂ condition. The morphology and compositions of CoRh₂O₄ and Co_xRh_{1-x} nanofibers were characterized by a field emission scanning electron microscope (FE-SEM) equipped with an energy dispersive X-ray spectrometer (EDS), high-resolution transmission electron microscopy (HR TEM) and X-ray photoelectron spectroscopy (XPS). The crystalline structures of the prepared nanofibers are investigated through high-resolution X-ray diffraction (XRD). Electrochemical activities for HER are studied with rotating disk electrode (RDE) voltammetry in N₂-saturated 1.0 M NaOH, 1.0 M PBS and 0.5 M H₂SO₄ aqueous solutions. This work was financially supported by the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT or by the Ministry of Education (NRF-2019R1F1A1059969, NRF-2020R1A2B5B01001984, NRF-2018R1A6A1A03025340, and NRF-2019R1F1A1062799).

Poster Presentation : **ELEC.P-810**

Electrochemistry

Zoom 20 FRI 16:00~17:00

Disposable capillary force driven-electrodynamic microfluidic heavy metal sensor

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Department of Chemistry, Pusan National University, Korea

A disposable electrodynamic microfluidic sensor was fabricated and demonstrated for the separation and detection of heavy metal ions. The electrodynamic capillary driven flow was controlled by the AC field applied on the microfluidic channel and the hydrophobisty of substrate. The microfluidic sensor was constructed using screen-printed carbon electrodes on a single platform composed of two parts on a plastic substrate; it includes a channel electrode for separation and a detection sensor in a three-electrode system (working, counter, and reference), where the detection electrode was mounted at the end of separation channel. To achieve the separation, the AC frequency applied on the channel wall and the capillary force were optimized. The working electrode surface of sensing part was modified with a conducting polymer of 3',4'-diamino-2,2'; 5'2"-terthiophene (pDATT)/nano-sized graphene oxide (GO) nanocomposite to sensitively detect heavy metal ions. The analytical parameters affecting the separation and detection of metal ions were optimized in terms of AC frequency, AC amplitude, flow rate, palstic substrate, pH, buffer concentration, temperature, and detection potential. The calibration plot reveals that the linear dynamic ranges are to be between 0.1 to 200.0 ppb and the lowest detection limits are determined to be 0.04 ± 0.023 , 0.29 ± 0.05 , 0.07 ± 0.011 , and 0.14 ± 0.06 ppb for Cu(II), Cd(II), Hg(II), and Pb(II), respectively. Finally, the device was applied to separately analyze heavy metal ions (Cu(II), Cd(II), Pb(II), and Hg(II)) in real water samples, which reveals that the results consistent with that using the conventional ICP-MS analysis at 96% confidence.

Poster Presentation : **ELEC.P-811**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Revisiting GITT Methods for Measuring Li⁺ Solid-state Diffusivity of LIB Electrodes by Simulation

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The solid-state diffusion of lithium ions (Li⁺) is the rate determining step for the operation of Li-ion batteries (LIBs). Galvanostatic intermittent titration technique (GITT) has been widely utilized to estimate the solid-state chemical diffusion coefficient D of Li⁺ in the electrodes. As this method assumes the linear dependence of the electrode potential and the depth of discharge (DoD), the plateaus in the two-phase reaction render significant uncertainties in the measurement of D . Herein we investigate the effects of the voltage profiles' shape on the accuracy of the D values from the above two equations. GITT data was generated by electrochemical simulation with a fixed solid-state diffusivity of $1.0 \times 10^{-10} \text{ cm}^2 \text{ s}^{-1}$ using the following models with varied complexity: a single particle model (SPM), an SPM with the dynamics of electrolyte, and a pseudo-two-dimensional (P2D) model. The electrochemical simulation involved various voltage profiles of single-phase and two-phase reactions. Afterwards, we compared the accuracy of the measured diffusivity with respect to the shape of the voltage profiles, shape of the electrode, and the level of the assumptions. This work points to the necessity of understanding the underlying principles for the meaningful estimation of the solid-state diffusivity by GITT.

Poster Presentation : **ELEC.P-812**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Stochastic Particle Approach Electrochemistry (SPAEC): Estimating Size, Drift Velocity, and Electric Force of Insulating Particles

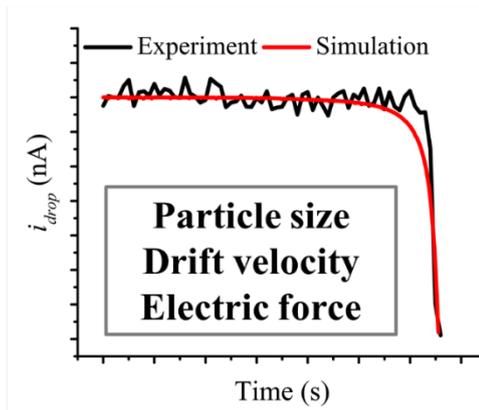
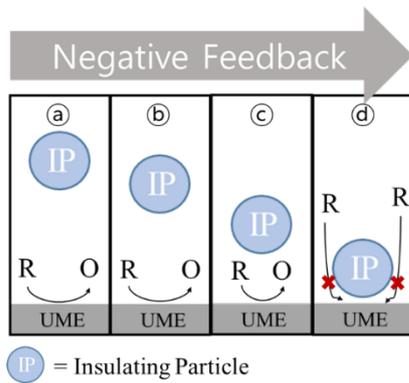
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Stochastic particle impact electrochemistry (SPIE) is considered one of the most important electro-analytical methods to understand the physicochemical properties of single entities. SPIE of individual insulating particles (IPs) has been particularly crucial for analyses of bioparticles. In this article, we introduce stochastic particle approach electrochemistry (SPAEC) for electrochemical analyses of IPs, which is the advanced version of SPIE; SPAEC is analogous to SPIE but focuses on deciphering a sudden current drop (SCD) by an IP-approach toward the edge of an ultramicroelectrode. Polystyrene particles (PSPs) with and without different surface functionalities ($-\text{COOH}$, $-\text{NH}_3$) as well as fixed human platelets (F-HPs) were used as IPs. From theory based on finite element analysis, a sudden current drop (SCD) induced by an IP during electro-oxidation (or reduction) of a redox mediator on a UME can represent the rapid approach of an IP toward an edge of a UME, where a strong electric field is generated. It is also found that the amount of current drop, i_{drop} , of an SCD depends strongly on both the size of an IP and the concentration of redox electrolyte. From simulations based on the SPAEC model that fit the experimentally obtained SCDs of three types of PSPs or F-HP dispersed in solutions with two redox electrolytes, their size distribution histograms are estimated, from which their average radii determined by SPAEC are compared to those from scanning electron microscopic images. In addition, the drift velocity and corresponding electric force of the PSPs and F-HPs during their approach toward an edge of a Pt UME are estimated, which cannot be addressed currently with SPIE. We further learned that we can provide a relative order of the excess surface charges on the IPs.

Stochastic Particle Approach Electrochemistry (SPAEC)



Poster Presentation : **ELEC.P-813**

Electrochemistry

Zoom 21 FRI 15:00~16:00

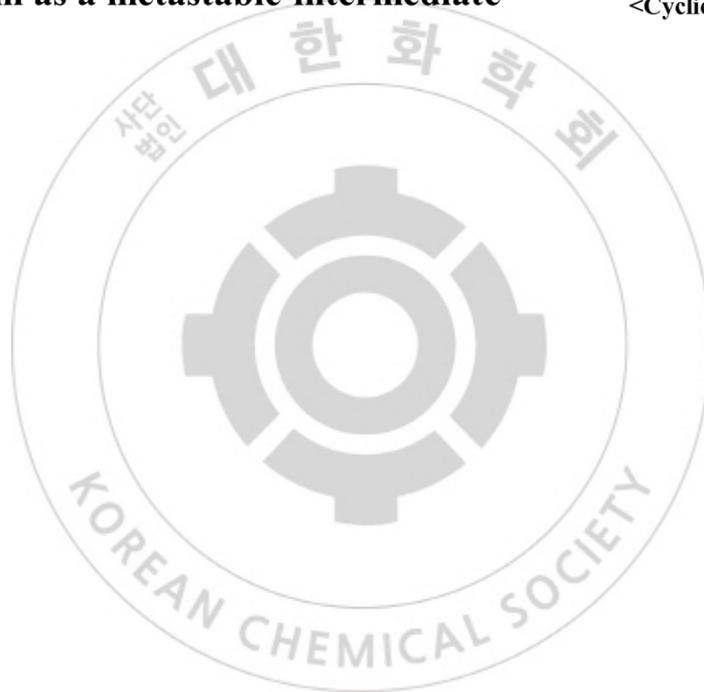
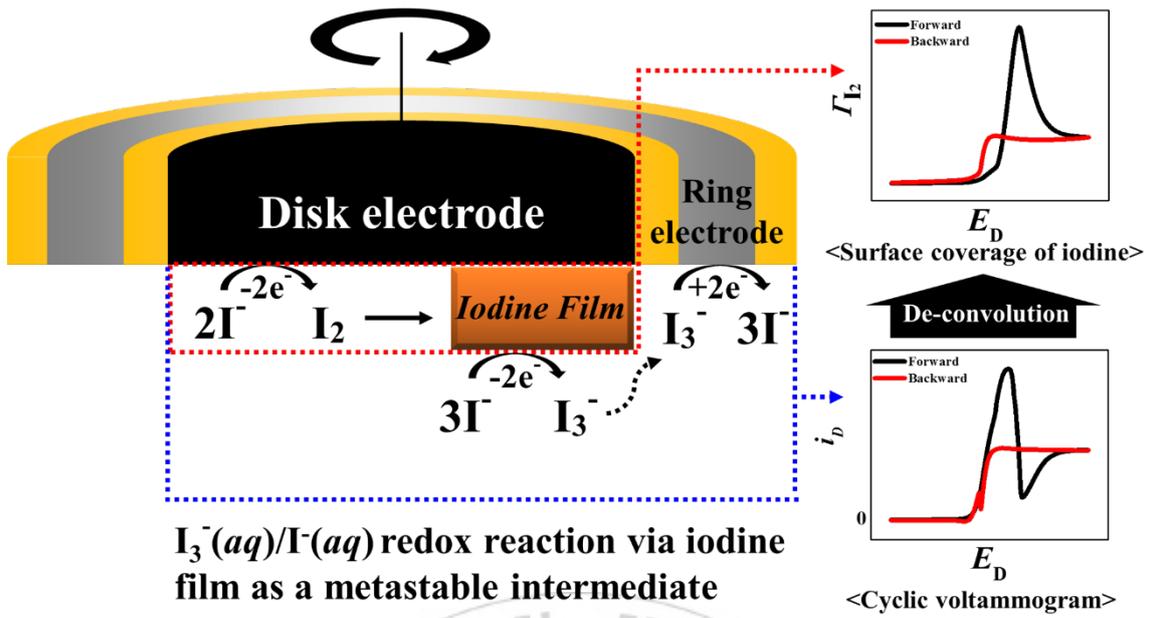
Electrochemical monitoring and mechanistic understanding of iodine film formation as a metastable intermediate during I_3^-/I^- redox reaction in aqueous ZnI_2 media.

Cheolmin Park, Jinho Chang^{1,*}

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Zn-polyiodide redox flow batteries (RFBs) are a promising grid-scale electrical energy storage (EES) option because of their significant energy density, which is due to the high solubility of ZnI_2 in water. In spite of the importance of the RFBs, a mechanistic understanding of both Zn^{2+}/Zn and I_3^-/I^- half redox reactions have not been fully achieved yet. The I_3^-/I^- half redox reaction occurring on a cathode in this RFB is particularly complicated due to metastable iodine films, which only form on an electrode when an electrochemical potential is biased enough to drive the electro-oxidation of I^- . The film is also difficult to characterize by ex-situ analyses, and its physicochemical properties are largely unknown. In this article, we report electrochemical in situ monitoring of a metastable iodine film as an intermediate during I_3^-/I^- redox reactions in an aqueous solution using a rotating ring disk electrode (RRDE). We suggested a reaction model for electro-oxidation of I^- to I_3^- via iodine films and its electro-reduction to I^- based on the mechanism proposed by Gileadi et al. Chronoamperograms (CAs) and cyclic voltammograms (CVs) associated with the I_2/I^- redox reaction involving only formation and dissolution of iodine films on a disk electrode were obtained using an RRDE. Then, we successfully obtained trajectory information on the formation and dissolution of an iodine film during the I_3^-/I^- redox reaction on a disk electrode under transient and potential-time variation conditions. In addition, we found evidence of a possible transition in the iodine film from an I^- -conductor to an I^- -semiconductor during formation based on the quantitatively monitored iodine formation curve as a function of time during electro-oxidation of I^- .



Poster Presentation : **ELEC.P-814**

Electrochemistry

Zoom 21 FRI 15:00~16:00

A Complete mechanism for Electrochemical oxidation of Serotonin on Glassy Carbon electrode by Cyclic Voltammetry

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We report the determination of a complete mechanism for electrochemical oxidation of serotonin (5-Hydroxytryptamine, SH₂) in a buffered condition with various pH using simulations of cyclic voltammograms on glassy carbon macroelectrodes at varying scan rates (0.02-1V/s). It has been reported the SH₂ is electro-oxidized to either S via 2H⁺-2e⁻ transfer (ECEC scheme) or SH⁺ via 1H⁺-2e⁻ (ECE scheme) in a neutral pH. By measuring Cyclic Voltammogram (CV) varying the pH in a universal buffer system and plotting E_{1/2} vs pH, we confirmed the electro-oxidation of SH₂ to S as ECEC scheme around neutral pH and there are some deviations at very low or very high pH. As scan rate for CV increases from 0.02 to 1V/s, it was observed that the voltammetric peak associated with electro-oxidation of SH₂ is gradually resolved into the two 1e⁻-1H⁺ transfers and we consider this would be mainly associated with kinetic difference between the first and second 1e⁻-1H⁺ transfer in SH₂/SH⁺ and SH⁺/S (so called kinetic discrimination). A complete reaction mechanism, including the elementary steps of each process, was fit to the voltammetric data using simulation software. In addition, about the deviations at very low or very high pH, by limiting the pathway we propose the oxidation mechanism of SH₂²⁺/SH₂ and S₂⁻/S.

Poster Presentation : **ELEC.P-815**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Modification of mediator and glucose dehydrogenase(GDH) onto the indium tin oxide electrode for continuous glucose monitoring

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Currently, in the glucose sensor market, Blood Glucose Meters (BGM) using disposable electrodes have been mainly used. Iron (Fe) based mediators, which are relatively inexpensive and have a good redox reaction, is one of the best candidate for BGM. However, in the case of the BGM sensor, when re-measurement is performed under the same electrode, there is a problem of showing a large error from the initial measurement. Recently, research on Continuous Glucose Monitoring (CGM), which solves this problem and monitors the blood sugar concentration in the body by measuring the blood sugar concentration continuously rather than repeating the measurement, is actively in progress. In this study, the mediator and glucose dehydrogenase were chemically modified to the electrode by covalent bonding with an epoxy functional groups rather than physical and electrical adsorption. To confirm the surface modification, we measured FT-IR. And the immobilization of the enzyme and mediator were characterized by HR-TEM, Raman, and EIS. And then we monitored the continuous glucose level by using I-t curve for 14 days. Finally, we observed the electrochemical currents about various glucose concentration through the chronoamperometry. This study is showing the stable immobilization of the mediator and enzyme onto the electrode. Also measurement of CGM was successfully achieved via electrochemical techniques. Therefore, we are expecting that our work can be applying to healthcare monitoring.

Poster Presentation : **ELEC.P-816**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Duplex Detection of Total and Active Enzyme Concentrations at a Single Working Electrode

Kyuseok Lee, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

It is still challenging that the duplex detection of both total and active enzyme concentrations without interferences at a single working electrode, especially when two different assays are combined. It is also difficult to obtain two different redox-cycling reactions without interference. In this paper, we show a simple but sensitive combined assay that is based on two redox-cycling reactions using two incubation periods and applied potentials at a single electrode. The assay combines an immunoassay for the determination of the total enzyme (total prostate-specific antigen, tPSA) concentration with a protease assay for the determination of the active enzyme (free PSA, fPSA) concentration. The immunoassay label and fPSA that are affinity-bound to the electrode are used for high sensitivity and specificity in the protease assay as well as the immunoassay. In the immunoassay, electrochemical-enzymatic (EN) redox cycling involving ferrocenemethanol is obtained at 0.1 V versus Ag/AgCl without incubation before the proteolytically released 4-amino-1-naphthol is generated. In the protease assay, EN redox cycling involving 4-amino-1-naphthol is obtained at 0.0 V after 30 min of incubation without ferrocenemethanol electro-oxidation. The detection procedure is almost the same as common electrochemical sandwich-type immunoassays, although the two different assays are combined. The duplex detection in buffer and serum is highly interference-free, specific, and sensitive. The limits of detection for tPSA and fPSA are approximately 10 and 1 pg/mL, respectively.

Poster Presentation : **ELEC.P-817**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Electrochemical Immunosensor Using an Enzymatic Cascade Reaction and a Redox Cycling Reaction

Gyeongsun Song, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

Horseradish peroxidase (HRP)-based electrochemical immunoassays are considered promising techniques for point-of-care clinical diagnostics, but the necessary addition of unstable H₂O₂ in the enzymatic system may hinder their practical application. Although glucose oxidase (GOx) has been widely explored for in situ generation of H₂O₂ in HRP-based immunoassay, the GOx-catalyzed reduction of oxidized peroxidase substrate may limit the immunosensing performance. Here, we report a sensitive electrochemical immunosensor based on a choline oxidase (ChOx)-HRP cascade reaction. In this design, ChOx catalyzes the oxidation of choline, during which H₂O₂ is generated in situ and thus oxidizes acetaminophen (APAP) in the presence of HRP. The electrochemical behavior of APAP in the ChOx-HRP cascade was compared with that of the commonly used GOx-HRP cascade, which confirmed that ChOx could be a superior preceding enzyme for sensitive immunoassay based on the enzymatic cascade. The developed ChOx-HRP cascade was also further explored for a sandwich-type electrochemical immunoassay of parathyroid hormone in artificial and clinical serum. The calculated detection limit was ~3 pg/mL, indicating that the ChOx-HRP cascade is especially promising for highly sensitive electrochemical immunoassays when APAP is used as the peroxidase substrate.

Poster Presentation : **ELEC.P-818**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Synthesis of Amine-Terminated Dendrimer-Encapsulated Pt Nanoparticles Using Galvanic Exchange

Jiwoong Kim, Joohoon Kim^{1,*}

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¹*Department of Chemistry, Kyung Hee University, Korea*

We previously reported decoration of graphene oxides (GOs) with Pt nanoparticles encapsulated in amine-terminated dendrimers (i.e., dendrimer-encapsulated Pt nanoparticles, Pt DENs) by covalent linkage of the terminal amine groups of the dendrimers for improved electrochemical oxygen reduction reaction.¹ However, when Pt DENs are synthesized by using only conventional chemical reduction, there is a drawback in that the size of Pt nanoparticles that can be formed inside the dendrimer is limited. In order to overcome this drawback, we also reported that larger sized of Pt nanoparticles could be synthesized inside a dendrimer having a hydroxy terminal functional group by a novel method combining chemical reduction and galvanic exchange.² Further from the previous studies, we herein intend to synthesize Pt DENs using amine-terminated dendrimers for a wide range of applications of Pt DENs using the terminal functional group. Pt DENs synthesized in this way can be decorated on the graphene oxides by utilizing the terminal amine groups of dendrimers.¹ *Chem. Commun.*, 2012, 48, 9233-9235² *Langmuir* 2018, 34, 7436-7444

Poster Presentation : **ELEC.P-819**

Electrochemistry

Zoom 21 FRI 15:00~16:00

DNA Detection Using Photoredox Catalysis Induced by Surface Plasmonic Field

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

Distance-dependent electromagnetic radiation and electron transfer have been commonly employed in washing free fluorescence and electrochemical bioassays, respectively. In this study, we combined the two distance-dependent phenomena for sensitive washing-free DNA detection. A distance-dependent surface plasmonic field induces rapid photoredox catalysis of surface-bound catalytic labels, and distance-dependent mediated electron transfer allows for rapid electron transfer from the surface-bound labels to the electrode. An optimal system consists of a chemically reversible acceptor ($\text{Ru}(\text{NH}_3)_6^{3+}$), a chemically reversible photoredox catalyst (eosin Y), and a chemically irreversible donor (triethanolamine). Side reactions with O_2 do not significantly decrease the efficiency of photoredox catalysis. Energy transfer quenching between the electrode and the label can be lowered by increasing the distance between them. Washing-free DNA detection had a detection limit of approximately 0.3 nM in buffer and 0.4 nM in serum without a washing step.

Poster Presentation : **ELEC.P-820**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Solid-Phase Isothermal Amplification for Sensitive Electrochemical Detection of Hepatitis B Viral DNA

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Recombinase polymerase amplification (RPA) is considered one of the best amplification methods for realizing a miniaturized diagnostic instrument; however, it is notably challenging to obtain low detection limits in solid-phase RPA. To overcome these difficulties, we combined solid-phase RPA with electrochemical detection and used a new concentration combination of three primers (surface-bound forward primer, solution reverse primer, and an extremely low concentration of solution forward primer). When solid-phase RPA was performed on an indium tin oxide (ITO) electrode modified with a surface-bound forward primer in a solution containing a biotin-terminated solution reverse primer, an extremely low concentration of a solution forward primer, and a template DNA or genomic DNA for a target gene of hepatitis B virus (HBV), amplification occurred mainly in solution until all the solution forward primers were consumed. Subsequently, DNA amplicons produced in solution participated in solid-phase amplification involving surface-bound forward primer and solution reverse primer. Afterward, neutravidin-conjugated DT-diaphorase (DT-D) was attached to a biotin-terminated DNA amplicon on the ITO electrode. Finally, chronocoulometric charges were measured using electrochemical-enzymatic redox cycling involving the ITO electrode, 1,4-naphthoquinone, DT-D, and reduced β -nicotinamide adenine dinucleotide. The detection limit for HBV was measured using microfabricated electrodes and was found to be approximately 0.1 fM. This proposed method demonstrated better amplification efficiency for HBV genomic DNA than solid-phase RPA without using additional solution primer and asymmetric solid-phase RPA.

Poster Presentation : **ELEC.P-821**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Simple Electrochemical Method for Investigating the Dissolution Behavior of Layers Deposited by Atomic Layer Deposition

Gyeongho Kim, Haesik Yang*

Department of Chemistry, Pusan National University, Korea

Spectroscopic and microscopic techniques are not suitable for the rapid monitoring of time-dependent dissolution behavior (particularly, pinhole changes) of a layer deposited by atomic layer deposition (ALD). Here, we present a simple electrochemical method that provides information on the dissolution mechanism including pinhole generation and thickness change. Because indium tin oxide (ITO) electrodes exhibit flat capacitive currents and good (electro)chemical stability, they are selected as ideal underlying substrates for the electrochemical monitoring of the ALD layers even under harsh conditions. Two ALD layers (Al₂O₃ and TiO₂ layers) that exhibit opposite dissolution behaviors are chosen as model layers because the as-deposited Al₂O₃ layers are pinhole-free but unstable in aqueous solutions, whereas the as-deposited TiO₂ layers are not pinhole-free but stable in aqueous solutions. The combination of capacitive current level (in an electrolyte solution containing no redox-active species) and electrochemical blocking behavior (in an electrolyte solution containing a redox-active species such as Ru(NH₃)₆³⁺ and ferrocenemethanol) obtained from cyclic voltammograms enables us to verify whether the dissolution of an ALD layer occurs, to evaluate the dissolution rate, and to identify the plausible dissolution mechanism. The electrochemical results reveal that the Al₂O₃ layers are dissolved in biological buffers, along with pinhole generation, and that the TiO₂ layers are stable with no pinhole generation. The difference in electrochemical blocking behavior between Ru(NH₃)₆³⁺ and ferrocenemethanol provides information on the approximate size of the pinholes. The present method is appealing for practical use because even an ALD layer with a thickness of only a few nanometers can be tested to monitor the dissolution behavior and because any ALD layer that can be readily deposited on ITO electrodes can be easily examined using this method.

Poster Presentation : **ELEC.P-822**

Electrochemistry

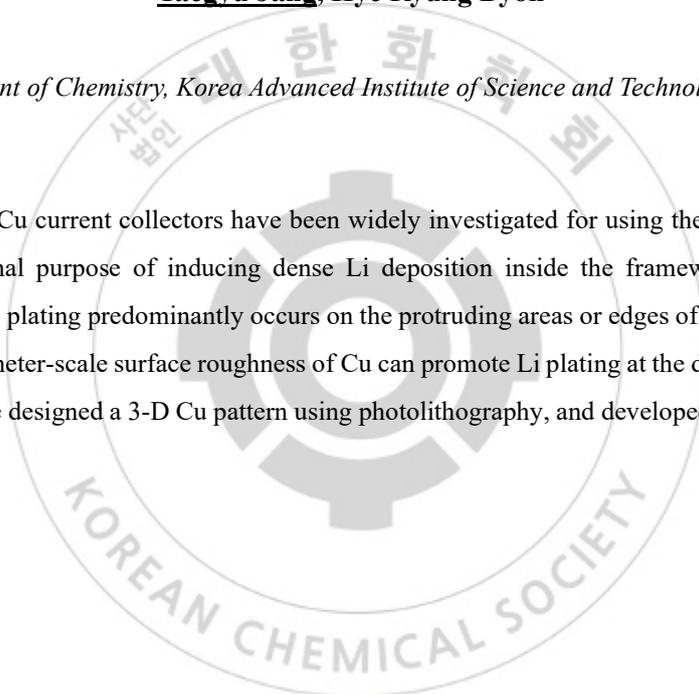
Zoom 21 FRI 15:00~16:00

Investigating a nanometer-scaled surface roughness effect of the Li electrodeposition in 3-D patterned Cu current collector for Li-metal batteries

Taegyu Jang, Hye Ryung Byon*

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Three-dimensional Cu current collectors have been widely investigated for using the Li metal electrodes. Despite their original purpose of inducing dense Li deposition inside the frameworks and mitigating dendritic growth, Li plating predominantly occurs on the protruding areas or edges of the top surface. Here we show that nanometer-scale surface roughness of Cu can promote Li plating at the desired position in the 3-D framework. We designed a 3-D Cu pattern using photolithography, and developed a receding area ~10 μm in depth with



Poster Presentation : **ELEC.P-823**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Solution structure change of Li-doped ionic liquid electrolytes induced by non-solvating diluent

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Energy Science & Engineering, DGIST, Korea

Room-temperature ionic liquids (RTILs) are promising electrolytes for Li-ion batteries due to their suitable properties including high electrochemical and thermal stability. In particular, recent studies reported reversible Li cycle performance in pyrrolidinium-based RTILs. However, RTILs suffer from high viscosity and thus poor transport properties. In this context, the co-use of low-viscosity diluent is an attracting approach to address the inherent issue of RTILs. In this study, the effect of highly fluorinated ether (HFE) as a diluent on the solution structure of N-methyl-N-propylpyrrolidinium bis(trifluoromethanesulfonyl)amide (PYR13TFSI) and N-methyl-N-propylpyrrolidinium bis(fluorosulfonyl)amide (PYR13FSI) with varying concentration of lithium salts (LiTFSI-PYR13TFSI and LiFSI-PYR13FSI) was investigated. To reveal the interaction among the ionic species, Raman spectroscopy, dielectric relaxation spectroscopy (DRS), and PFG-NMR were employed. It is found that the solution structure of LiFSI-PYR13FSI is hardly altered by the presence of HFE, whereas structure alteration of LiTFSI-PYR13TFSI is caused by the presence of HFE. This change occurs from separation of PYR13 cation, which was originally engaged to lithium coordination structure.

Poster Presentation : **ELEC.P-824**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Revealing origins of product selectivity in Cu-based electrocatalysts during CO₂ reduction reaction via operando electrochemical scanning transmission x-ray microscopy

Ju Won Kim, Yun Jeong Hwang^{1,*}, Jongwoo Lim^{2,*}

Department of Chemistry, Seoul National University, Korea

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²*Division of Chemistry, Seoul National University, Korea*

Carbon capture and utilization (CCU) is drawing attention around the world as a way to solve the problem of greenhouse gas emission and increasing energy demand. Among various efforts, the conversion of CO₂ into fuels and value-added chemicals via electrochemical methods is a representative technology of CCU. Using Cu-based electrocatalysts for CO₂ reduction reaction (CO₂RR), CO₂ can be converted into hydrocarbon compounds. Especially, C₂ products are known to provide high energy density with larger global markets compared to C₁ products. The oxide-/hydroxide-derived Cu electrocatalysts can achieve high activity and selectivity toward C₂ products. Since electrocatalysts generally undergo dramatic phase transformations, it remains very difficult to correlate the activity with the chemical structure of catalysts at action. While it has been widely hypothesized that the presence of Cu¹⁺ phase or morphological deformation/evolution during CO₂RR could lead to the enhanced C-C coupling reaction, the experimental evidences are rarely demonstrated. In this work, we developed operando electrochemical scanning transmission x-ray microscopy (STXM) to image compositional(i.e. Cu, Cu¹⁺, Cu²⁺) and morphological evolutions during CO₂RR. STXM is a synchrotron-based x-ray microscopy which sensitively images oxidation states at nanometer scales. Owing to the superior sensitivity, our unprecedented results clearly reveal that Cu¹⁺ chemical composition in oxide-/hydroxide- derived Cu electrocatalysts persists during CO₂RR. In addition, we discover that the dynamic morphology evolution is strongly correlated with C-C coupling enhancement. This study demonstrates that operando chemical imaging can aid in investigating electrocatalysis mechanism and designing the efficient CO₂RR catalyst.

Poster Presentation : **ELEC.P-825**

Electrochemistry

Zoom 21 FRI 15:00~16:00

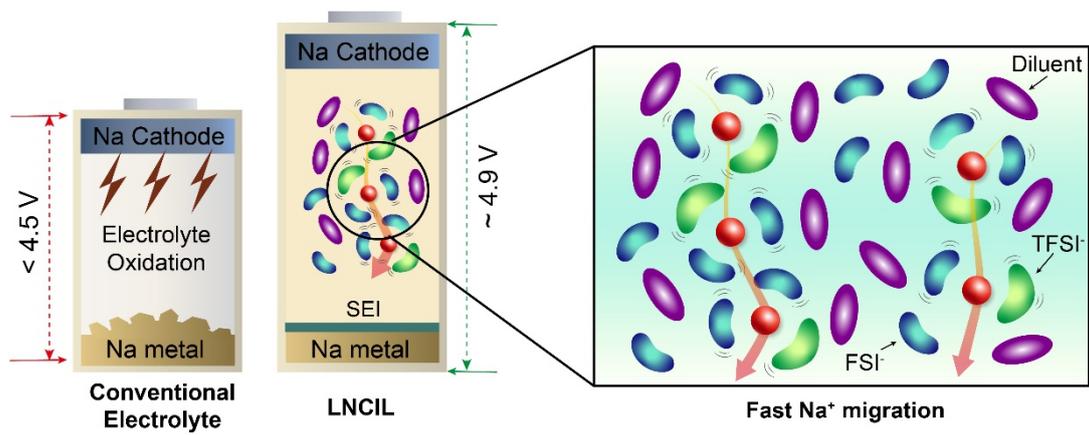
Localized Sodium Ion Concentrated Ionic Liquid Electrolyte for Safe, High-Voltage Sodium-Metal Batteries

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Sodium (Na)-powered rechargeable batteries (NRBs) are promising as sustainable energy storage systems. To overcome an inherent energy density handicap of NRBs, increasing cell voltage is necessary by building a Na metal battery (NMB), which simultaneously features coveted high-voltage stability and efficient Na dendrite protection. Although ionic liquids (ILs) are eligible to provide superior oxidative stability, their practical uses are challenging due to high viscosity and sluggish ionic transport at a higher Na concentration. Here, a localized Na⁺ ion concentrated ionic liquid (LNCIL) electrolyte consisting of an IL and a hydrofluoroether (HFE) as cosolvents is developed. The addition of a non-solvating HFE lowers the viscosity and improves separator wettability, thereby facilitating Na⁺ ion transport. Furthermore, HFE dilution promotes the involvement of dual anions (FSI/TFSI) in the development of a protective solid-electrolyte interphase, leading to Na dendrite suppression. A Na||Na₃V₂(PO₄)₃ cell incorporating the LNCIL electrolyte demonstrates excellent cyclability (~96.6% capacity retention over 500 cycles). Moreover, with oxidative stability up to 4.9 V (vs. Na/Na⁺) and non-flammability, the LNCIL electrolyte ensures the safe operation of high-voltage NMBs.



Poster Presentation : ELEC.P-826

Electrochemistry

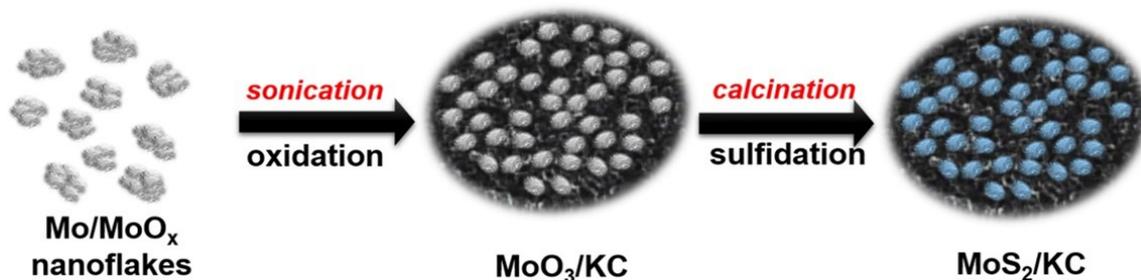
Zoom 21 FRI 15:00~16:00

Non-Noble Metal Molybdenum Disulfide Electrocatalysts for Oxygen Reduction Reaction

Youchang Park, Kang Hyun Park*

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The oxygen reduction reaction (ORR) is currently recognized as a significant process in the energy conversion and storage field. We introduce a facile method for synthesizing carbon-supported noble metal-free catalysts using molybdenum species. These molybdenum oxide nanoparticles around 3 nm were well dispersed on the carbon support materials (MoO₃/KC). After the sulfidation of MoO₃/KC, the prepared MoS₂/KC showed improved activity derived from the synergistic effects of the metal and chalcogenide atoms compared to MoO₃/KC toward the ORR. Chronoamperometric analysis demonstrated the excellent durability of these molybdenum nanocatalysts compared with that of Pt/C. Furthermore, MoS₂/KC was not affected by methanol, where the linear sweep voltammetry (LSV) curve remained the same before and after methanol injection. The stability and methanol tolerance of these nanocatalysts suggest their possibility for replacing Pt/C catalyst in energy areas such as direct methanol fuel cells (DMFCs) on account of benefits of low-cost and simple synthesis.



Poster Presentation : **ELEC.P-827**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Development of chemical oxygen demand determination system in a boron-doped diamond thin layer cell

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Traditional water analysis and treatment methods, such as Chemical Oxygen Demand (COD), are carried out based on homogeneous chemical oxidation of organic molecules. However, the use of expensive and toxic chemicals as the oxidizing reagents can lead to secondary waste production. The advanced electrochemical oxidation process (AEOPs) is considered an appealing approach to overcome concerns associated with the conventional COD since it removes the need for chemical oxidants. It can also provide a rapid and straightforward COD determination method by employing a specially designed thin-layer cell using a boron-doped diamond (BDD) electrode. Numerous electrochemical applications utilize boron-doped diamond as the anode material due to its unique properties such as wide potential window, low background current, and resistance to fouling. The employment of BDD for anodic oxidation of organics enables a direct oxidation of the molecules via electron transfer taken place at the anode surface or indirect oxidation via physically adsorbed hydroxyl radicals ($\bullet\text{OH}$) which offers a high standard redox potential of $E^\circ(\bullet\text{OH}/\text{H}_2\text{O}) = 2.80 \text{ V/SHE}$. As an electrochemical oxidant, $\bullet\text{OH}$ has a high reactivity towards organics degradation and a short lifetime, makes it possible to be utilized for the on-site electrochemical oxidation process. By this means, this study aims to develop an electrochemical system for COD determination. The quantification of COD value will be measured based on the amount of electron transferred at the BDD thin-film electrode. A 300 μm thick silicon rubber is used as a spacer. The assay time of less than three minutes can be achieved for a series of samples containing analytes within a range of 10-100 ppm. Higher concentrations of organic compounds require a longer time to decay, thus resulting in higher COD values. The major experimental conditions of the anodic oxidation of organic molecules by BDD, such as applied potential bias, supporting electrolyte concentration, and pH, will also be studied to obtain the optimum conditions.

Poster Presentation : **ELEC.P-828**

Electrochemistry

Zoom 21 FRI 15:00~16:00

Iridium metal nanowires as electrocatalyst for oxygen evolution reaction

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¹*Department of Applied Chemistry, Kumoh National Institute of Technology, Korea*

Hydrogen-based energy has become an excellent solution for unreliable carbon-based energy. The excess energy from photovoltaic system can be utilized by electrolyzer to break the water into hydrogen and oxygen. In the electrolysis process, oxygen evolution reaction (OER) in anode requires higher energy than hydrogen evolution reaction (HER) in cathode. Iridium has low overpotential and has been known as the most stable electrocatalyst for OER yet the most expensive one. Thus, an effective, durable, and inexpensive electrocatalyst is necessary to overcome this issue. To suppress the cost and enhances the electrocatalytic activity, iridium metal nanowires are fabricated by galvanic displacement. Non-platinum group metal (PGM) nanowires such as Ag, Cu, Ni, and Co are used as base metal, and they are coated with iridium by galvanic displacement synthesis. The electrocatalytic activities of those iridium metal nanowires are compared with Ir-black. In conclusion, iridium metal nanowires are promoted to have better performance and more affordable than Ir-black.

Poster Presentation : **ELEC.P-829**

Electrochemistry

Zoom 21 FRI 15:00~16:00

In situ synthesis of single atom nickel catalysts for enhanced electrochemical CO₂ reduction

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Department of Chemistry, Pusan National University, Korea

Electrochemical CO₂ reduction (ECR) provides a useful source of valued hydrocarbons, and it is a promising approach to reduce CO₂ levels. However, poor product selectivity is still a major obstacle to the development of ECR. In addition, the stability of the catalysts during electrolysis is of great significance. Here we report facile synthesis of glassy carbon electrode on an alumina plate, and consecutive synthesis of a single atom nickel catalyst on the glassy carbon electrode (Ni SAC-GC). The Ni SAC-GC electrode exhibited excellent activity for ECR with particularly high selectivity, achieving high faradaic efficiency over 90% for CO in the potential range from -0.65 V to -1.35 V and gives a maximum faradaic efficiency 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 strong electrode that are suitable for industrial application.

Poster Presentation : **EDU.P-830**

Chemistry Education

Zoom 19 FRI 16:00~17:00

A Study on the Improvement of Teaching Professionalism through the Practical Education Program Based on Technology Utilization of Pre-service Chemistry Teachers.

Misun Jung, Seounghey Paik*

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

This study was conducted to investigate the improvement of TPACK(Technological Pedagogical Content Knowledge) through the process of planning and executing a class program utilizing technology of pre-service chemical teachers. The participants of this study were 20 third graders and 2 fourth graders of chemistry education at K University in Chungcheong province. The TPK(Technological Pedagogical Knowledge) of the participants before the program was classified into three levels, and the TCK(Technological Content Knowledge) was all identified as low. For this study, the researcher conducted a class to analyze and discuss the phenomenon and model of the chemistry-related unit of middle school science and high school integrated science, and then introduced various technology programs and practice time was given. And, as part of the practice-based education program, the teaching and learning program using technology was demonstrated to students by utilizing the teaching-learning period, and the educational results were presented and the questionnaires were analyzed to understand the improvement of TPACK. The researchers divided the utilization level of technology into three stages: transparent technology, user technology, and maker technology, considering the interaction with students. In the final stage of the class, the researcher examined the perception of the technology utilization class program through essay questionnaires.

Poster Presentation : **EDU.P-831**

Chemistry Education

Zoom 19 FRI 16:00~17:00

Analysis of pre-service teachers' TPACK development type and factors that hinder the development

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¹*Department of Chemical Education, Korea National University of Education, Korea*

In this study, to determine the practical competency development of pre-service teacher TPACK, based on previous research, we developed a TPACK development assessment rubric from level 0 to level 4. Based on the technology-using class design submitted by pre-service teachers, the TPACK competency was analyzed. The factors that hindered the development of TPACK of the pre-service teachers were investigated through the feedback submitted after the pre-service teachers observed the class rehearsal using technology. The analysis showed that most pre-service teachers had the same level of TPK, TCK and TPACK. However, for some pre-service teachers, the level was unbalanced because the TPK level was higher than the TCK level or vice versa. In this case, the TPACK step was found to follow the lower step of the TPK step and the TCK step. Also, as the TPACK of pre-service teachers develops, it is shown that the initiative of manipulation, exploration and learning goal are sequentially transmitted from teachers to students. On the other hand, the negative beliefs of pre-service teachers that can hinder the development of TPACK appeared to be distrust of the student's self-regulated learning ability, the effect of communication between students, and practical limitations in the school field.

Poster Presentation : **EDU.P-832**

Chemistry Education

Zoom 19 FRI 16:00~17:00

**the Analysis of changes in pre-service secondary science teachers'
perceptions toward character education in science teaching using
Collaborative Problem-Solving for Character competence (CoProC)
instruction model**

Jihun Park, Jeonghee Nam^{1,*}, Kim Hyunjin

Pusan National University, Korea

¹*Department of Chemical Education, Pusan National University, Korea*

The purpose of this study was to investigate the changes in the perception toward character education of preservice secondary school science teachers by applying the Collaborative Problem-Solving for Character competence (CoProC) developed as the practice of character education in science education to science classes. The sixteen participants were chosen among the attendees in courses(lectures) related to science inquiry experiment offered in chemistry education of college of education in busan. The participants took part in the two-period of workshops about CoProC model and character education and the demonstration of group CoProC instruction for six months. Pre-questionnaires and post-questionnaires about the perception toward character education, interviews, recordings of three-period of classes during the courses were collected and analyzed. A researcher conducted an unstructured interview for deep understanding about questionnaires.

Poster Presentation : **EDU.P-833**

Chemistry Education

Zoom 19 FRI 16:00~17:00

Identification and investigation about the level of modeling in the states of matter targeting inservice and preservice teachers

Yunji Nam, Seounghey Paik*

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

The purpose of this study was to identify the level of modeling of graduate students majoring in chemical education through modeling classes on the state of matter and to conduct training for 15 weeks to change their perception to find out the educational effects. Participants in the study were eight graduate students of the Department of Chemical Education at K University in Chungcheong Province. For this study, we identified the initial perception of the model of expressing the state of matter in the first phase of the class(week 1-3). After then the participants analyzed the units related to the state of matter in middle school science and high school chemistry textbooks(week 4-6). The textbook and curriculum were reconstructed, considering the characteristics of the model regarding the state of matter(week 7-11). The participants also used technology to refine the model by representing the model related to the state of the material they thought of and comparing it to the phenomenon. In the final phase of the class(week 15), the participants examined the perception of modeling and modeling using technology about the states of matter. The responses of the participants were analyzed using a coding scheme consisting of three steps, comparing problem solutions and epistemic practices.

Poster Presentation : **EDU.P-834**

Chemistry Education

Zoom 19 FRI 16:00~17:00

A Study on the Improvement of Collaborative Mentoring Program for Enhancing Teaching Expertise of Beginning Science Teachers.

Hyo Jung Ryu, Jihun Park, Jeonghee Nam^{1,*}

Pusan National University, Korea

¹Department of Chemical Education, Pusan National University, Korea

This study aims to find out how to improve the collaborative mentoring program for enhancing teaching expertise of beginning science teachers. Using survey data which were collected from teachers who participated in the collaborative mentoring program from 2016 to 2020, a total of 74 surveys participants' perception of collaborative mentoring program were analyzed. The survey questionnaire consisted of multiple-choice and short answer questions to find out opinions on 'the way of operating collaborative mentoring program and the contents of its activities, the overall perception of mentors and mentees on collaborative mentoring, and the introduction of online course in the program'. In addition, four mentors and four mentees were selected from the teachers who participated in the survey and interviewed for an in-depth understanding of the survey result. Moreover, it was possible to find ways to improve the collaborative mentoring program from the previous studies on mentoring.

Poster Presentation : **EDU.P-835**

Chemistry Education

Zoom 19 FRI 16:00~17:00

Study on Evaluation Questions in Chemistry I textbooks and College Scholastic Aptitude Test by Bloom's New Taxonomy of Educational Objectives

Heesu Sim, HyunJu Park^{1,*}

Chemistry Education, Chosun University, Korea

¹*Faculty of Chemistry Education, Chosun University, Korea*

The purpose of this study was to investigate evaluation questions in chemistry I of textbooks and college scholastic aptitude test by Bloom's new Taxonomy of Educational Objectives. A total of 570 evaluation questions were analyzed to Bloom's new taxonomy of educational objectives. As results, 'Factual knowledge', 'conceptual knowledge' in the dimension of knowledge, 'remember' in the dimension of cognitive processes were mainly presented in evaluation questions in chemistry I of textbooks and college scholastic aptitude test.

Poster Presentation : **EDU.P-836**

Chemistry Education

Zoom 19 FRI 16:00~17:00

Analysis of Social Emotional Learning (SEL) Elements in 2015 Revised Science Curriculum Achievement Standards and Textbooks

SeoYoung Kim

Chosun University, Korea

The purpose of this study was to investigate the Science Social Emotional Learning elements on the 2015 revised science curriculum and the achievement standards and science textbooks, and suggests in educating social emotional learning in science education. The subjects of the study were a total of 139 achievement standards of required science courses such as middle school science, integrated high school science, and science inquiry experiments, and science activities in textbooks for those required courses. The analysis unit was organized as follows: an achievement statement of national curriculum, and one inquiry activity. The elements of Science Social Emotional Learning included in each analysis unit were analyzed. The collected data were analyzed by arithmetic statistics including frequency.

Poster Presentation : **EDU.P-837**

Chemistry Education

Zoom 19 FRI 16:00~17:00

Acid-base neutralization experiment using IoT technology

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The problem of not being able to conduct experiments in non-face-to-face classes inevitably in the Pandemic Era due to Coronavirus 19 (COVID-19). Indirect experimental methods, such as watching experimental videos and simulating demonstrations, can not be directly manipulated by the experimental performers, or only pre-designed experimental results can be presented. In this study, we recognize the current situation and create a new experimental device with non-face-to-face methods. IoT-based neutralization-appropriate experimental devices developed in this study can conduct experiments such as manipulating experimental devices and deriving results by experimental performers in real time. In other words, the developed experimental device can utilize Arduino and wireless Internet-based IoT applications and conduct acid-base neutralization experiments by conditioning a quantifiable liquid pump motor. Furthermore, the experimental performers are expected to be able to conduct the experiments with safety in the experimental equipment and spaces different from the situation. Therefore, we would like to propose this research method to conduct direct experiments in the current non-face-to-face life. This study was conducted with the funding of the Ministry of Education with the support of the Korea Research Foundation.(No. 2019S1A5A2A03051489)

Poster Presentation : **EDU.P-838**

Chemistry Education

Zoom 19 FRI 16:00~17:00

Light Synthesis Device Using AI Speech Recognition

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¹Department of Chemistry Education, Korea National University of Education, Korea

As the era of artificial intelligence arrives, science departments also need to develop scientific exploration activities using artificial intelligence. This study aims to combine existing maker education activities with AI speech recognition to provide students with scientific exploration activities using AI. Microcontrollers such as Arduino and Microbit, which are used in traditional maker training, are not insufficient to control sensors and actuators, but are limited to installing artificial intelligence programs or libraries. Therefore, this work performs light synthesis experiments in middle school curriculum by mounting Google Assistant, an AI voice recognition tool, and controlling General port input/output (GPIO) pins in Raspberry Pi, a Unix-based compact computer. The device is configured as follows: Raspberry Pi 4B+, Microphone, 3 RGB_LEDs, Bread board, Jumper cables. Google Assistant, an AI voice assistant, is installed on Raspberry Pi and the Python program is used to modify the code in the Pushtalk.py file to add commands. The three RGB_LEDs emit seven different light colors, red, green, blue, magenta, yellow, turquoise, and white, depending on the coding of the added voice command. This allows students to conduct light synthesis experiments using AI speech recognition. If the conventional light synthesis experiment only synthesized three lights of red, green, and blue to observe and confirm the three primary colors of light, students can try various light synthesis, share it with each other, and find the three primary colors of light by themselves. This work, utilizing AI speech recognition light synthesis devices, will improve existing light synthesis experiments and contribute to connecting AI to science by giving students the experience that AI technology can also be applied to scientific exploration activities.

Poster Presentation : **EDU.P-839**

Chemistry Education

Zoom 19 FRI 16:00~17:00

Molecular structure learning tool making exploration activity using AI image recognition

SoRim Her, Seong-Joo Kang^{1,*}

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¹Department of Chemistry, Korea National University of Education, Korea

There is a growing interest in AI in many fields, and the need for education using AI is emerging in the field of education as well. AI education is mainly conducted in nonsubject, and there are not many examples of education using AI in science subject. Therefore, it aims to provide educational opportunities to use AI in science subject to prospective teachers in a changing era. AI technologies include image, voice, and text recognition. In this study, an activity to make a molecular structure learning tool that can give feedback using image recognition was organized. Prospective teachers add AI image recognition technology to the existing molecular structure making exploration activities to create learning tools that can give feedback on the molecular structure students are making. We used Teachable Machine as AI tool and Kami Block based on scratch as coding tool. Prospective teachers generate image data on molecular structures with a webcam, machine learning to AI, and execute script actions through coding. In this process, prospective teachers understand the principle of image recognition, experience AI tools firsthand, and implement a flow chart with coding. In this study, we expect that the AI value awareness and AI efficacy of prospective teachers will increase, and we intend to provide them with educational opportunities to use AI in science subject.

Poster Presentation : **ENVR.P-840**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Photo-induced process on TiO₂@graphite-derived carbon dot through ligand-to-metal charge transfer

Hoang Tran Bui

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The combination of nano-sized TiO₂ and carbon materials for energy and environmental applications has been studied and renovated frequently in the present. These materials consume the visible light effectively and perform the superior photocatalytic properties. The ligand-to-metal charge transfer conception (LMCT) is an alleged mechanism of the visible-light activation of TiO₂-carbon material composites. Nonetheless, the direct evidence of LMCT band formation is rarely described in detail in published researches. Herein, we synthesized TiO₂@graphite-derived carbon dot and employed this composite in order to interpret the LMCT process between nano-sized TiO₂ and graphene-derived carbon dots (GCDs) under visible illumination. The contribution of GCDs on TiO₂ activity enhancement is inspected through the hydrogen peroxide generation and pollutant degradation (organic, e.g. 4-chlorophenol and inorganic compound, e.g. hexavalent chromium). Our study provides decisive proof for the LMCT mechanism of TiO₂@GCD, which is expected to strengthen the understanding of this composite.

Poster Presentation : **ENVR.P-841**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Preparation of Dimensionally Stable Electrodes Using Titanium Substrates

Jong-Hyeok Park, Jin-Soo Park^{1,*}

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¹*Department of Green Chemical Engineering, Sangmyung University, Korea*

Recently, electrodes technology is being intensively developed for a variety of energy conversion devices which could use spontaneous or unspontaneous reactions. Developed electrode technology allows us to apply for all of the reversible or even irreversible reactions in a view of energy conversion such as fuel cell, water electrolysis, carbon organics synthesis from carbon dioxide, degradation of non-degradable organic compounds which are not possible to perform when they are carried out by biochemical technology. Particularly, discharge of the industrial wastewater has been significantly increased due to industrial development and that will be a serious cause of water pollution. There are various water treatment technologies such as chemical oxidation, precipitation, adsorption, capacitive deionization, electrochemical oxidation and so on. Electrochemical oxidation of the compounds at anode is environmentally friendly, easily operated and maintained compared to conventional treatment processes. Nonetheless, cost reduction and enhancement of performance/durability of anodic electrodes are highly necessary for commercialization. In this study, TiO₂/IrO₂/RuO₂ electrodes that IrO₂ and RuO₂ coated on anodized Ti substrate were prepared and investigated in terms of various electrochemical properties. Acknowledgment This research was supported 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).

Poster Presentation : **ENVR.P-842**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Glycol Based Ionomer Dispersions for Catalyst Layers in Proton Exchange Membrane Fuel Cells

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¹*Department of Green Chemical Engineering, Sangmyung University, Korea*

Fuel cells require the movement of ions generated and consumed at two electrodes, i.e., anode and cathode. Ions should be transported inside electrodes to participate in anodic and cathodic reactions. Much efforts have been devoted to develop quasi-solid electrolytes such as gel polymer, ion exchangeable polymers, impregnation of ions in porous matrix and so on. Among the candidates, ion exchangeable polymers are quite often chosen as ion conducting media for energy conversion devices. The technique to introduce ion exchangeable polymers within electrodes for oxidation and reduction reactions is to solidify catalyst inks consisting of electrocatalyst, dispersion of ion exchangeable polymers, controlling solvents and additives by evaporation of all solvents in catalyst inks. Ion exchangeable polymers could be dispersed in various solvents. It causes different shapes of ion exchangeable polymers in solvents, for instance, cylindrical rods, a less-defined large particles, coils and so on. Such different types of ion exchangeable polymers form distinguished structure catalyst layers. In this study, the effect of solvents dispersing ion exchangeable polymers 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. Acknowledgment This work was supported 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).

Poster Presentation : **ENVR.P-843**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Direct observation of intermediates on Pt electrode for electrocatalytic oxidation of ammonia

Hong Phuc Dinh

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

Elucidating the profound reaction pathway of ammonia electrocatalytic oxidation on Pt surface is a key to the successful introduction of the nitrogen energy cycle, which is one of the most promising source for hydrogen fuels. Although various mechanisms were already reported, the dominant effect of poisoning species which caused the significant deactivation on Pt surfaces during ammonia oxidation process still roughly interpreted. Herein, nanofilm platinum layer electrodeposited on the gold chemically fabricated electrodes were employed for thoroughly study of electrooxidation of ammonia in alkaline solution by conducting time-solved attenuated total reflection-surface enhanced infrared absorption spectroscopy (ATR-SEIRAS) associated with cyclic voltammetry and chronoamperometry measurements. These results provide a physical insight into the detriment of Pt metal that could be used as a guideline for further development of efficient ammonia oxidation to close the nitrogen cycle.

Poster Presentation : **ENVR.P-844**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Hg-contaminated sediment remediation by mechanochemically sulfidated microscale zero valent iron

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

¹*Division of Environmental Engineering, Pohang University of Science and Technology, Korea*

Mercury (Hg) contamination in sediment is a significant concern to the environment and public health due to the production of toxic methylmercury (MeHg) via methylation of inorganic divalent mercury (Hg(II)). However, the effective in-situ remediation of Hg-contaminated sediments remains a technological challenge. Mechanochemically sulfidated microscale zero valent iron (S-mZVI^{bm}) is one of the most fascinating soil and groundwater remediation materials due to its high removal efficiency of toxic metals and amenability to up-scaling. The objective of this study is the remediation of Hg-contaminated anoxic sediment using S-mZVI^{bm}, investigating the fate of Hg in microcosm. The study tested sediment slurry microcosms that are each amended with three different materials: mZVI^{bm}, FeS^{bm}, and S-mZVI^{bm}. To gain insight into the underlying Hg remediation mechanisms, we are probing any change in soil-bound Hg speciation, gaseous Hg(0) generation, and net MeHg production.

Poster Presentation : **ENVR.P-845**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Optimization of Fenton oxidation of methyl orange by olivine/ hydroxylamine/ hydrogen peroxide system

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In this study, various natural Si/Al minerals containing a few amount of Fe_2O_3 (i.e., olivine, elvan, sericite, zeolite, and loess) were used for enhanced Fenton oxidation of methyl orange (MO) at pH 3. Hydroxylamine (HA, NH_2OH) and hydrogen peroxide (H_2O_2) were applied as a reduction agent for Fe(III) to Fe(II) and an oxidation agent for OH radical production, respectively. Among the minerals, olivine/HA/ H_2O_2 system shown the highest removal of MO was selected as a main system in this study. In addition, the concentration effects of olivine, HA, and H_2O_2 were investigated, which revealed the increase of rate constant (i.e., k fitted by first-order reaction) as increasing the concentrations, except the case of high dosage of H_2O_2 . RSM analysis was done to find out the optimal reaction condition, showing the optimal concentrations of 7.5 mM HA, 7.5 mM H_2O_2 , and 0.5 gL^{-1} olivine. Mechanical studies revealed that the Fenton oxidation of MO by olivine/HA/ H_2O_2 system was mainly induced by a homogeneous Fenton reaction owing to the Fe ions dissolved from the olivine suspension, and HA played a key role in the enhanced MO removal in this study. Acknowledgments: This research was supported by the National Research Foundation of Korea (2019R1C1C1003316).

Poster Presentation : **ENVR.P-846**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Removal of hexavalent chromium by nanoscale zerovalent iron supported by natural zeolite (NZVI@Zeolite)

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Nanoscale zerovalent iron (NZVI) is one of the potential materials, which could be applied in in-situ remediation of soil and groundwater because of its small particle size, high surface area, and high reactivity. However, the high surface energy and magnetic interaction properties of NZVI induce particle agglomeration, consequently reducing the reaction surface area and clogging soil pores, limiting their injection into the soil. Therefore, the severe inhibition of aggregation of NZVI is a key parameter to increase its activity and application, and one of the solutions is the use of the support material such as zeolite. In this study, we developed NZVI@Zeolite using a natural zeolite (i.e., Clinoptilolite) as support material for preventing agglomeration of NZVI. From the sedimentation test, it was confirmed that the developed NZVI@Zeolite could be dispersed for a long time in a stable colloidal state compared to the Bare NZVI, and the column study showed 90% particle could flow out without blocking the soil column. A variety of surface analysis such as X-ray diffraction, scanning electron microscope, and Fourier transform infrared were carried out to characterize the NZVI@Zeolite. Finally, we applied the NZVI@Zeolite for reductive removal of hexavalent chromium (Cr(VI)), showing the remarkable reactivity toward Cr(VI). The results of this study highlight the potential applicability of natural zeolite as a supporting material for in-situ remediation nanomaterials of soil and groundwater contaminated with Cr(VI). Acknowledgments: This research was supported by the Korea Environment Industry & Technology Institute (KEITI) through "Subsurface Environmental Management (SEM) Project", funded by Korea Ministry of Environment (MOE) (2020002480006)

Poster Presentation : ENVR.P-847

Environmental Energy

Zoom 22 FRI 15:00~16:00

Various Geometric Design of Anodic 1D TiO₂ Nanotube Arrays for the Electrochemical reduction of 2,4,6-Trinitrotoluene under Ambient Condition

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In this work, we demonstrated the various geometric design of anodic 1D TiO₂ nanotube (NT) arrays for their electrochemical reduction performance of 2,4,6-trinitrotoluene (2,4,6-TNT) in the aqueous solution under the ambient condition. TiO₂ NTs were fabricated by anodization of Ti foil in four different composition of fluoride-contained organic solvents. Anodically formed TiO₂ NTs samples were successfully detected the 2,4,6-TNT in the aqueous solution via cyclic voltammetry (CV) method; with three reduction peaks corresponding to each nitro groups on 2,4,6-TNT in the potential range from -0.5 to -1.0 V (vs. Ag/AgCl (3 M KCl)). We revealed that the detection of 2,4,6-TNT reduction are depended on tube length. Additionally, we performed for various scan rates and limit of detection; the optimum geometry to clear detection of 2,4,6-TNT was 75±5 nm of inner diameter and 6 μm of tube length. Through the various scan rates, we also observed that the 2,4,6-TNT cathodic reduction was occurred by dominating diffusion as the mass transfer. Limit of detection of selected electrode was determined as 5 ppm with linear range (5-100 ppm).

Poster Presentation : **ENVR.P-848**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Synthesis of anodic spaced TiO₂ nanotubes / BiVO₄ heterojunction to enhance photoelectrochemical efficiency

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Recently, research on sustainable eco-friendly energy production has been actively conducted to solve the problem of excessive energy consumption and greenhouse gas emission. Hydrogen energy has been considered one of the best energy resources due to high energy efficiency per unit mass clean with zero emission of pollutant such as CO₂, CO, and NO₂ etc. To produce hydrogen various methods are conducted such as petrochemical byproduct hydrogen, hydrocarbon reforming and photoelectrochemical water splitting etc. Among them, PEC water splitting is in the spotlight because it does not emit pollutants. TiO₂ is the promising material for PEC electrode due to good physical and chemical stability and cheap. However, it has a relatively large bandgap energy of 3.0 to 3.2 eV that allows absorbed UV light less than 400nm of wavelength. In order to overcome drawbacks formation of heterojunction with lower bandgap energy materials such as BiVO₄, WO₃, and α -Fe₂O₃ has been studied. In particular, BiVO₄ absorbs light in the visible range of less than 563 nm with a low band gap of 2.2 to 2.4 eV and excellent stability, so it can be expected to increase the photoelectrochemical efficiency. In this work, we designed a spaced TiO₂ nanotubes / BiVO₄ heterojunction to enhance the photoelectrochemical efficiency. The spaced TiO₂ nanotubes allows to coat BiVO₄ thin films onto inner and outer wall at the nanotubes, that lead to improving photoelectrochemical efficiency due to the large surface area.

Poster Presentation : **ENVR.P-849**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Formation of Ni₂S₃ / NiO Heterostructures to improve water electrolysis performance

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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-based materials have been attracted attention as a promising water electrolysis catalyst. In our research group, Ni₂S₃/NiO heterostructures were fabricated by hydrothermal and electrodeposition method.

Poster Presentation : **ENVR.P-850**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Moth eye inspired SiO₂ nano structure Via polystyrene nanosphere lithography for anti-reflective surfaces

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Natural creatures have various optical properties; among them, the moth's eye has a low-reflective structure. Moth-eye inspired structures have increased surface transmitted light compared to planar ITO/Glass. The amount of transmitted light increases due to the gradual decrease in the refractive index. Applying moth eye low reflective properties, moth-eye mimicking structures were fabricated in a hexagonal-closed packed array on glass on an ITO deposition substrate using polystyrene (PS) nanosphere lithography (NSL) and reactive ion etching (RIE). The diameter of the PS mask was adjusted using O₂ gas, and the height of SiO₂ was adjusted using CHF₃ gas. Through this selective etching process, it was possible to fabricate SiO₂ moth-eye structures. To maximize the anti-reflection effect for visible light, 98 nm of MgF₂ was deposited. The measurement results for our moth-eye structure (Diameter: 165 nm, Height: 400 nm) showed a 2.89 % reflectance reduction in the visible wavelength (380~780 nm) compared to that of planar ITO/Glass substrate. To obtain self-cleaning surface characteristics, self-assembled monolayer (SAM) treatment was performed on the SiO₂ moth-eye structures. A field emission scanning electron microscope (FE-SEM) was used to measure the morphology of the SiO₂ moth-eye structures. The moth-eye structure can be applied to places requiring low reflection, such as photovoltaics, lasers, light-emitting diodes, and windows.

Poster Presentation : **ENVR.P-851**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Atmospheric moisture effect on deactivation process for VOCs degradation under UV-illuminated TiO₂.

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Volatile organic compound (VOC) has affected a number of air pollution problem, Especially, it is toxic for indoor air quality even at small concentrations. Accordingly, photocatalysis technology has been extensively applied with development of LED technology for efficient treatment of VOCs. TiO₂ has been investigated as the primary photocatalyst for removing VOCs with economic benefits and sufficient oxidation power. However, the problem of deactivation of the catalysts remains as unsolved problem. The degree of deactivation depends on the structure of VOCs, and in this work, the chain-type structure of acetaldehyde (C₂H₄O) and ring-type toluene (C₇H₈) were selected to explain the difference as representative materials. Furthermore, the effect of atmospheric moisture on catalytic activity was observed. It is related to removal efficiency about both substances and has particularly influence on the mineralization of toluene. In this research, we investigated about relationship between photodegradation behavior of the VOCs and atmospheric moisture based on real-time Fourier transform-infrared (FTIR) analysis. Research of real-time changes with moisture in these VOCs photodegradation reactions can identify the cause of instability of catalysts, which can offer a basis to propel real-life application of photocatalytic technology for removing the harmful VOCs for safe air quality.

Poster Presentation : **ENVR.P-852**

Environmental Energy

Zoom 22 FRI 15:00~16:00

CO₂ reduction using a composite photocathode of CuFeO₂@CuO semiconductor with rGO, PPy layers.

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Global warming is one of the serious environmental issues that creates many disasters, including heat waves, floods, storms, and droughts. [Ref 1] Among some greenhouse gases in the atmosphere, CO₂ is considered as one of the most critical climate change gas. Photoelectrochemical (PEC) 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-layer electrode FTO/CuFeO₂/CuO/rGO/PPy/Nafion has been prepared as a photocathode for a smooth and effective CO₂ reduction with FTO@BiVO₄ as a anode. A composite of p-type semiconductors, CuFeO₂@CuO has chosen for CO₂ reduction because of its narrow bandgap for visible light absorption and conduction band position which is suitable for CO₂ reduction energy level. [Ref 2,3,4] The material PPy has selected to adsorb and activate a highly stable CO₂ molecule. By considering the multi electron, CO₂ reduction reaction for useful products rGO layers have been introduced into cathode electrode. [Ref 5] A 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-853**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Improved operation stability of perovskite solar cells via heat dissipation and morphology fixation

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Perovskite solar cells (PSCs) are promising energy harvesting applications owing to remarkable high power conversion efficiency. However, the instability of perovskites at high temperatures impedes the practical use of PSCs. We, for the first time, find that great heat absorption in the perovskite layer occurs, leading to thermal decomposition. This is one of the main reasons for the efficiency drop in PSCs, but an increase in temperature is inevitable during the operating condition. To solve this issue, it is essential that fast heat pumping from the inner side (perovskite layer) of a device to the surrounding area should be realized. Therefore, we introduce Al₂O₃-infiltrated hole-transporting materials to eliminate the heat continuously accumulated in the device, which adversely affects the performance of solar cells. To confirm the effect of heat dissipation and morphology fixation, we designed the stability test similar to the real operating environment. As a result, we demonstrate a highly stable planar PSC retaining 91% of its initial efficiency for 31 days under a harsh condition without encapsulation.

Poster Presentation : **ENVR.P-854**

Environmental Energy

Zoom 22 FRI 15:00~16:00

Enhancement of photovoltaic properties of perovskite solar cells with novel cathode Interfacial layer using creatine

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The interlayers of perovskite solar cells (PSCs) passivate traps on the surface, help to extract the charge smoothly, and shift the energy level, contributing many roles to the development of PSCs. In addition, these can also improve the stability of PSCs. Herein, we introduce a small molecular self-assembled monolayer (2-[carbamimidoyl(methyl)amino]acetic acid) on a SnO₂ layer. The acetic acid is known as creatine, which is naturally present in the human body. It can be eaten and dosed by athletes for energy. Due to its structural properties, creatine can be anchored on a SnO₂ layer, thus improving charge extraction in the perovskite layer by forming an interfacial dipole and reducing the work function. In addition, it can effectively passivate the defects in the perovskite layer. As a result, PSCs with creatine layer exhibited improved power conversion efficiency (PCE) of 22.1% and excellent stability, maintaining 90% of a maximum efficiency after 50 days. This study demonstrated an interesting application in the field of perovskite solar cells as an interlayer of creatine and the applicability of other essential amino acids.

Poster Presentation : **ENVR.P-855**

Environmental Energy

Zoom 22 FRI 16:00~17:00

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

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Burn-in loss in ternary blended organic photovoltaics (OPVs) manufactured by a UV-crosslinkable semiconducting polymer (P2FBTT-Br) and a nonfullerene acceptor (IEICO-4F) using a green solvent process, was studied in this work. 150 seconds of UV irradiation were used to crosslink the synthesized P2FBTT-Br and 2-methylanisole were used to dissolve it with its asymmetric structure. In OPV test for performance and burn-in loss executed at 75 °C or AM 1.5G Sun illumination for 90 h, UV-crosslinked devices with PC71BM exhibited 9.2% power conversion efficiency (PCE) and better stability on burn-in loss compared to the pristine devices. The anchored morphology from the crosslinking prohibits lateral crystallization and aggregation leading to morphological degradation. When IEICO-4F was introduced as a substitute for the fullerene-based acceptor, the burn-in loss brought by the temperature and light was effectively suppressed due to the anchored morphology and high miscibility of the nonfullerene acceptor (18.7% → 90.8% after 90 h at 75 °C and 37.9% → 77.5% after 90 h at AM 1.5G). The resulting crosslinked device exhibited 9.4% PCE (9.8% in chlorobenzene), the highest value in crosslinked active materials using the green processing approach.

Poster Presentation : **ENVR.P-856**

Environmental Energy

Zoom 22 FRI 16:00~17:00

High performance Halogenated Small Molecule Organic Solar Cells via Bulk-heterojunction Morphology Control

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Tuning excellent bulk-heterojunction (BHJ) architecture is a key factor which determined the efficiency of organic solar cells. Halogenated benzodithiophene(BDT)-based active materials were developed to control the BHJ architecture. BDT and PC71BM are blended and this BHJ morphology are analyzed using grazing-incidence wide-angle X-ray scattering (GIWAXS). The chlorine substituted BDT (BDTID-Cl) exhibits an excellent morphology and interpenetrating networks which resulting an efficient charge transportation. From this approach, 10.5% power conversion efficiency (PCE) and the highest fill factor of 78.0% in the single-junction organic solar cells. Moreover, PCE of 15.1% is achieved via two-terminal(2T)-tandem solar cells.

Poster Presentation : **ENVR.P-857**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Morphological engineering of thermally stable organic solar cells using highly miscible semiconducting polymer

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The development of thermal stability is still crucial requirement in the multi-functional organic solar cell technology. Tailoring the morphology of semiconducting polymers driving and thermal stability is a key factors. Herein, we demonstrate a multi-functional organic solar cell with the addition of an asymmetric NDI-based polymer (asy-PNDI1FTVT) to a PTB7-Th/Y6 blend system. The asy-PNDI1FTVT has remarkably lower crystallinity than symmetric poly-mers (PNDITVT, PNDI2FTVT) in GI-WAXS results owing to the asymmetric structure. The hypermiscibility of asy-PNDI1FTVT in PTB7-Th:Y6 is present near the percolation threshold, which exhibited a well-intercalated morphology at the bulk heterojunction, and efficiently facilitated the charge dissociation process with enhanced FF and power conversion efficiency (PCE). Furthermore, the ternary system of PTB7-Th:asy-PNDI1FTVT:Y6 showed a PCE of 12.5%, and high miscibility of asy-PNDI1FTVT suppresses the phase separation of blend system, resulting in negligible burn-in loss (at 75 °C for 400 h).

Poster Presentation : **ENVR.P-858**

Environmental Energy

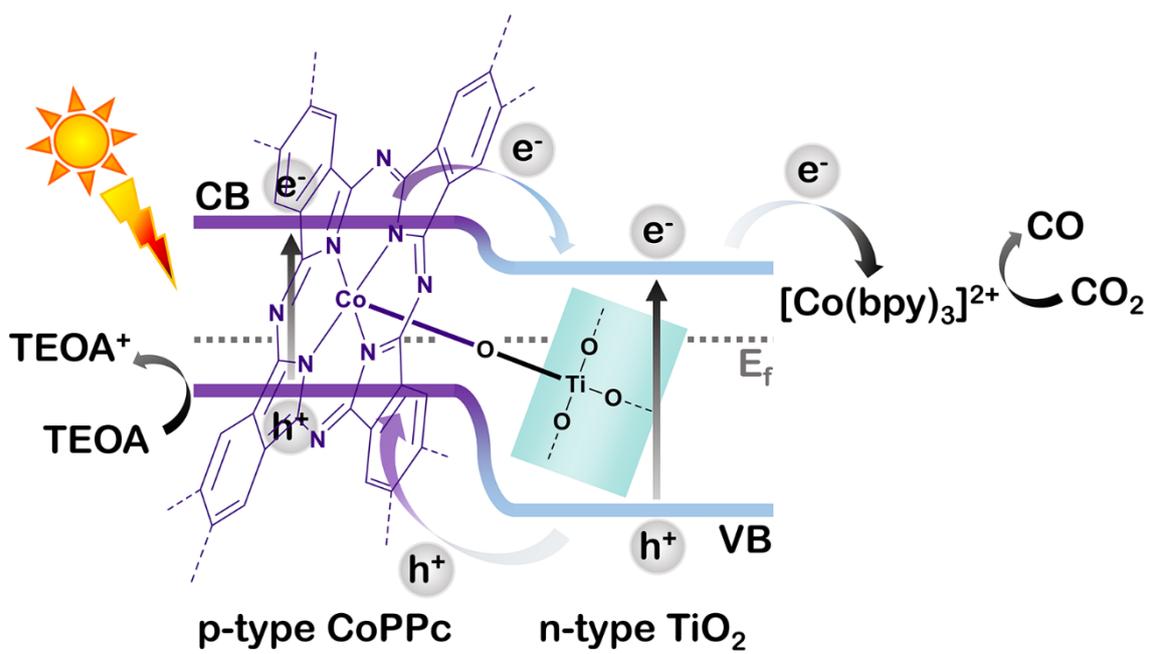
Zoom 22 FRI 16:00~17:00

In-situ Preparation of Polymeric Cobalt Phthalocyanines Decorated TiO₂ Nanorods for Efficient Photocatalytic CO₂ Reduction

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The integration of photosensitizers with low-cost, and non-toxicity metal oxides is a promising strategy to design heterogeneous photocatalysts for CO₂ reduction. In this study, polymeric cobalt phthalocyanines (CoPPc) as the photosensitizer were supported on TiO₂ nanorods through a facile one-pot hydrothermal reaction. A p-n heterojunction with the strong interfacial contact of the nanohybrid allowed efficient carrier transport and recombination suppression. In addition, the enhanced solar light utilization contributed significantly to the improvement in the photocatalytic performance. The CO₂ photoreduction of the synthesized materials was evaluated in CO₂-saturated MeCN/water using [Co(bpy)₃]²⁺ as a cocatalyst and TEOA as a hole scavenger. The optimized nanocomposite exhibited a remarkable CO generation rate of 4.42 mmol·h⁻¹·g⁻¹ with high selectivity of 85.3 % and outstanding catalytic stability. The influences of cocatalyst concentration, water content, catalyst loading, and hole scavenger concentration were optimized for effective CO₂ reduction. The photocatalytic CO₂ conversion efficiency of the present system is found to be higher than that of TiO₂ based materials reported in the literature. We believe that the heterostructure design strategy and the photocatalytic system may bring inspiring research for the development of photocatalytic CO₂-to-CO conversion.



Poster Presentation : **ENVR.P-859**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Selective Nitrogen Reduction under Neutral pH Condition using Mo oxide decorated Rh electrocatalyst

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Electrochemical nitrogen reduction reaction (NRR) has drawn significant attention as an alternative route for green ammonia production due to single step process, low energy consumption in comparison with the traditional Haber-Bosch process. In this study, a molybdenum oxide decorated rhodium electrocatalyst (RhMoOx/C) is fabricated using an electrodeposition technique. With the dual active sites of Mo and Rh for nitrogen reduction reaction, the RhMoOx/C electrode shows a higher yield of ammonia and higher faradaic efficiency in comparison with the pristine Rh/C electrode. Moreover, the operation under neutral pH conditions successfully inhibited the hydrogen evolution reaction (HER) which is the competing reaction against the electrochemical ammonia synthesis. This study reveals the relationship between the reaction condition and the selectivity of ambient ammonia synthesis.

Poster Presentation : **ENVR.P-860**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Surface proton assisted electrochemical NH₃ synthesis using carbon nanofiber based CoMo bimetallic catalyst

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Ammonia (NH₃), one of the important chemicals in the global economy, is generally used for the production of fertilizers, refrigerants and other chemical feedstocks. Ammonia is also being considered as an effective carbon-free energy carrier due to its' high density of hydrogen. Haber-Bosch process which is the main route for ammonia synthesis, requires huge energy consumption. As an alternative route for green ammonia production, electrochemical method for ammonia synthesis at ambient conditions has been recently received much attention. In this study, different ratio of cobalt (Co), molybdenum (Mo) bimetal embedded carbon nanofiber (CoMo-CNF) electrocatalysts were synthesized using an electrospinning technique. With the strong hydrogen evolution reaction (HER) activity of Co and the strong affinity of nitrogen on Mo, the amount of proton was controlled on the surface of carbon nanofiber. This study reveals the important role of surface proton in electrochemical NH₃ synthesis on the bimetal embedded carbon nanofiber catalysts.

Poster Presentation : **ENVR.P-861**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Enhanced Electrochemical Ammonia Synthesis on RuO₂ by Amphiphilic Ionic Liquid

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Ammonia has received great attention as a promising energy storage medium and a fuel on behave of hydrogen gas, which has some issues of transportation and storage. However, the production of ammonia is limited to only Haber-Bosch process, which consumed 2 % of the global annual energy and generated 0.5 % of the CO₂ emission. Recent studies showed the feasibility of electrochemical ammonia production by the reduction of abundant N₂ gas in ambient pressure and temperature using metal electrocatalysts such as Ru, Rh, and, Fe. But, the Faradaic efficiency for nitrogen reduction reaction (NRR) is only ~1 % due to both very close theoretical potential with hydrogen evolution reaction (HER) and difficult N₂ adsorption on the catalyst compared with proton. Here, we fabricated well-dispersed RuO₂ powder on carbon fiber by amphiphilic ionic liquid for electrochemical ammonia synthesis. The ionic liquid consisting of imidazole and hydroxyl ion helped the dispersion of RuO₂, which increased electrochemically active surface area. Furthermore, imidazole in the ionic liquid scavenged the adsorbed proton at negative potential so that RuO₂ can adsorb the nitrogen molecule for facile NRR rather than HER. The two roles of ionic liquid can enhance both ammonia production rate and Faradaic efficiency at low negative potential compared with pristine RuO₂ catalyst.

Poster Presentation : **ENVR.P-862**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Photocatalytic CO₂ reduction on reduced TiO₂ via magnesiothermal synthesis

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Elevated atmospheric CO₂ levels have been recognized as a key driver of global warming. Making use of sunlight to photoreduce CO₂, in turn fabricating hydrocarbon fuels compatible with the current energy infrastructure, is a promising strategy to minimize atmospheric CO₂ concentrations. However, practical application of such a photocatalytic system requires significant efforts for improved photoreduction performance and product selectivity. Herein, we investigate the performance of our newly developed reduced TiO₂, prepared by a reduction process using Mg in 5% H₂/Ar, for photoconversion of CO₂ and water vapor to hydrocarbons, primarily CH₄. Using Pt nanoparticles as a co-catalyst, under simulated solar light irradiation the reduced anatase TiO₂ exhibits a relatively stable performance with a threefold increase in the rate of CH₄ production (1640.58 ppm g⁻¹ h⁻¹, 1.13 μmol g⁻¹ h⁻¹) as compared to anatase TiO₂ nanoparticles (546.98 ppm g⁻¹ h⁻¹, 0.38 μmol g⁻¹ h⁻¹). The improved photocatalytic performance is attributed to enhanced light absorption, suitable band edge alignment with respect to the CO₂/CH₄ redox potential, and efficient separation of photogenerated charges. Our results suggest that the Pt-sensitized reduced TiO₂ can serve as an efficient photocatalyst for solar light CO₂ photoreduction.

Poster Presentation : **ENVR.P-863**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Heterostructured hybrid $\text{Cu}_x\text{O-TiO}_2$ composites for photocatalytic CO_2 Reduction into Methane

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Photocatalytic CO_2 conversion to fuel offers an exciting prospect for solar energy storage and transportation thereof. Several semiconductor photocatalysts have been employed for CO_2 photoreduction; the challenge of realizing a low-cost, readily synthesized photocorrosion-stable photocatalytic material that absorbs and successfully utilizes a broad portion of the solar spectrum energy is as yet unmet. Herein, a mesoporous p-type/n-type heterojunction material, $\text{Cu}_x\text{O-TiO}_2$ ($x = 1, 2$), is synthesized via annealing of $\text{Cu/Cu}_2\text{O}$ nanocomposites mixed with a TiO_2 precursor (TiCl_4). Such an experimental approach in which two materials of diverse bandgaps are coupled provides a simultaneous opportunity for greater light absorption and rapid charge separation because of the intrinsic p-n heterojunction nature of the material. As detailed herein, this heterostructured photocatalyst demonstrates an improved photocatalytic activity. With the CO_2 reduction of our optimal sample (augmented light absorption, efficacious charge separation, and mesoporosity) that utilizes no metal cocatalysts, a remarkable methane yield of $221.63 \text{ ppm}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ is achieved.

Poster Presentation : **ENVR.P-864**

Environmental Energy

Zoom 22 FRI 16:00~17:00

A noble metal-free hybrid Z-scheme Cu₂ZnSnS₄ (CZTS)-ZnO for enhanced photocatalytic conversion of CO₂ to CH₄

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Development of photocatalytic materials for achieving the aspects of cost-effectiveness, improved performance and high stability is a subject of enormous interest among the photocatalysis research society. With the aim of achieving above mentioned features, herein we report a noble metal free, solar-light active, efficient and highly stable hybrid Cu₂ZnSnS₄ (CZTS)-ZnO photocatalyst, synthesized by a simple two-step process. The morphological, crystalline, band alignment, optical and electronic properties of the prepared samples are intensively investigated. Photocatalytic performance is evaluated by measuring, under the simulated solar light, the ability of the photocatalyst to convert CO₂ into hydrocarbon fuels, primarily CH₄. Our optimum CZTS-ZnO photocatalyst sample exhibits a CH₄ yield of 138.90 ppm g⁻¹ h⁻¹, a factor of ≈ 31 times greater than the un-sensitized ZnO nanorods, and ≈ 22 times greater than the CZTS nanoparticles; with excellent stability yielding similar CH₄ production up to five test-cycles. The enhanced performance of the hybrid, noble metal-free photocatalyst can be attributed to improved light absorption and efficient separation of the photogenerated charge due to the Z-scheme heterojunction interface.

Poster Presentation : **ENVR.P-865**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Heterojunction p-n-p Cu₂O/S-TiO₂/CuO to photocatalytic conversion of CO₂ to CH₄

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Photocatalytic conversion of CO₂ to fuel is one of great current interest. The problem is a challenging one, requiring a stabile, industrially-scalable, broad light-absorbing semiconductor, the energy bands of which align with the CO/CO₂ and H₂O/O₂ potentials. Herein we report the synthesis of a unique p-n-p heterojunction material architecture, Cu₂O/S-doped TiO₂ micro-blocks covered with CuO nanowires, using anodization and annealing processes. The photocatalytic material shows excellent performance in the photocatalytic conversion of CO₂ and water vapor to CH₄ under AM 1.5G illumination. The heterojunction material architecture exhibits a methane yield of 2.31 μmol m⁻² h⁻¹, a rate approximately ten times higher than TiO₂ nanotube array films.

Poster Presentation : **ENVR.P-866**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Facile fabrication of a noble metal-free photocatalyst: TiO₂ NTs covered with rGO

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TiO₂ nanotubes arrays (TNT) are the subject of great current interest among the photocatalysis research, however the relatively large bandgap that provides TiO₂ with its excellent corrosion stability severely limits its absorption of solar spectrum energy. To increase the optical absorption of TiO₂ while maintaining its otherwise commendable properties a number of 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, herein 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-TiO₂ nanoparticles (rGO-TiO₂ NP) composite. The novel nanostructure exhibits significantly improved photocurrent density and photochemical activity via conversion of CO₂ into methane under simulated solar light irradiation. The improved performance appears due to the combined effect of enhanced light absorption and effective charge separation promoted by the rGO.

Poster Presentation : **ENVR.P-867**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Optimal Functional Group Pairing of Polymer Donor/Small-Molecule Acceptor for High-Performance Organic Solar Cells

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The recent development of non-fullerene small molecule acceptors (SMAs) has enabled a significant improvement of the power conversion efficiency (PCE) of organic solar cells (OSCs). As increasing the diversities of SMAs, pairings with optimal polymer donors (PDs) is an important issue. Herein, a systematic investigation is conducted with the development of a series of SMAs, named as C6OB-H, C6OB-Me, and C6OB-F, which contain distinctive terminal substituents -H, -CH₃, and -F, respectively. Interestingly, the PD/SMA pairs with similar terminal groups yield enhanced molecular compatibility and energetic interactions at the interfaces, which suppress voltage loss while improving blend morphology to simultaneously enhance the open-circuit voltage, short-circuit current, and fill factor of the OSCs. This study establishes an important PD/SMA pairing rule in terms of terminal functional groups for achieving high-performance OSC with optimal blend morphology, effective charge generation, and minimal voltage loss.

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Environmental Energy

Zoom 22 FRI 16:00~17:00

C70-based Aqueous-Soluble Fullerene Acceptors for Eco-Friendly Organic Solar Cells with Water Ratio-Tolerant Efficiencies

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Eco-PSCs based on alcohol-soluble conjugated materials have recently received great attention. In this work, a new alcoholic solvent-processable C70-based fullerene (PC71BO15) is reported. The PCEs of PC71BO15-based eco-PSCs up to 2.5%, which is the top number for aqueous-processed PSCs, was achieved. At the best fabrication condition, the PCE of the PC71BO15-based eco-PSCs is 73% higher than that of the PC61BO15-based counterparts, as a result of enhanced photon absorption. More importantly, the PC71BO15-based eco-PSCs show much greater tolerance in their PCEs to the solvent blending ratio. PC71BO15-based eco-PSCs at a 30% water ratio maintain 89% of the optimal efficiency at a 15% water ratio. Different aggregation behaviors induced large difference in terms of water ratio-tolerant behavior, which is systematically studied by electrical, optical and morphological characterizations. The PC71BO15-based eco-PSCs is able to have excellent reproducibility due to the great water content-tolerance.

Poster Presentation : **ENVR.P-869**

Environmental Energy

Zoom 22 FRI 16:00~17:00

Synthesis and Characterization of Oligothiophene-fullerene Integrated Triads for Single-Component Organic Solar Cells

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Organic solar cells (OSCs) have attracted large attention for last several decades on their applicability for portable electronic devices with good processability upon large-area and flexible substrate. As a result of development of material design and fabrication techniques, bulk-heterojunction (BHJ) OSCs succeeded to achieving the excellent power conversion efficiencies over 17%. The optimized morphology on BHJ films with appropriate donor/acceptor interpenetrating networks can provide efficient charge separation of excitons and transportation for energy harvest. However, it is hard to get the optimum of nano-phase morphology of BHJ films and it also can be easily changed and degraded upon their fabrication and working conditions such as temperature, blend ratio and post-treatment, which also directly affects to the stability of the OSCs. As a novel strategy to simplifying the fabrication conditions and stabilizing the morphology of the OSCs, single-component (SC) molecules can be adopted, which the donor and acceptor moieties are integrated by a covalent linkage. In this study, we designed and synthesized the new oligothiophene-fullerene integrated triad SC photoactive materials by modulating the length of σ -spacers to optimize the morphology and charge transfer properties. The synthesis of new materials and their optical, morphological, electrical and photovoltaic properties will be presented in detail.